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MCNPX EXTENSIONS
VERSION 2.5.0

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Abstract

MCNPX is a Fortran90 Monte Carlo radiation transport computer code capable of tracking 34 particle types at nearly all energies. It is a superset of MCNP4C and MCNPX2.3.0. This document describes the capabilities beyond these constituent codes.

1.0. INTRODUCTION

MCNPX is a Fortran90 (F90) Monte Carlo radiation transport computer code that transports 34 particle types, including 4 light ions, at nearly all energies. MCNPX stands for MCNP eXtended. It is a superset of MCNP4C3 and MCNPX2.3.0 and has many capabilities beyond these constituent codes. These capability extensions enhance physics, sources, tallies, graphics, and infrastructure.

MCNPX is a production computer code for modeling the interaction of radiation with matter, and its quality is guaranteed. See Section 1.2 about the MCNPX guarantee and cash awards. MCNPX is widely used around the world. See Section 1.3 for availability.

MCNPX is backward compatible with MCNP4C3 and older MCNPX (2.3.0 and earlier) versions. Old input files still work and usually track, giving identical results. The new MCNPX capabilities involve some changes, but mostly extensions, to the input cards

1.1. MCNPX Extensions

Each successive version of MCNPX adds new capabilities and modernizes the code for new hardware, operating systems, and compilers. The extensions of MCNPX beyond MCNP4C and MCNPX2.3.0 now are listed with the initials of the principal developers shown in parentheses.[1] Section 9 contains a complete list of new capabilities since MCNP4B was grouped according to version release.

Physics

- Mix and match (JSH);
- CEM2k physics (SGM/AJS/FXG);
- INCL4/ABLA physics models (JCD/JSH);

[1] Kenneth J. Adams (KJA), Nate A. Carstens (NAC), Leland L. Carter (LLC), Skip Egdorf (HWE), Thomas M. Evans (TME), Jeffrey A. Favorite (JAF), Franz X. Gallmeier (FXG), John S. Hendricks (JSH), H. Grady Hughes (HGH), Julian Lebenhaft (JL), Robert C. Little (RCL), Stepan G. Mashnik (SGM), Gregg W. McKinney (GWM), Eric J. Pitcher (EJP), Richard E. Prael (REP), Teresa L. Roberts (TLR), Arnold J. Sierk (AJS), Edward C. Snow (ECS), Avneet Sood (AS), Martyn T. Swinhoe (MTS), Laurie S. Waters (LSW), Christopher J. Werner (CJW), and Morgan C. White (MCW).

- Extension of neutron model physics below 20 MeV (JSH);
- Fission multiplicity (JSH);
- Light-ion recoil (JSH);
- Inline generation of double differential cross sections and residuals (JSH);
- Photon Doppler broadening (from MCNP5) (AS/GWM);
- Weight-window generator and exponential transform for model physics (FXG/ JSH); and
- Improved S(α,β) physics (RCL/EJP).

Sources

- Spontaneous fission (JSH);
- Multiple source particle types (JSH/MTS);
- Repeated structures source-path improvement (LLC/JSH);
- Positron sources (HGH);
- Sources on cylindrical surfaces (GWM/JSH); and
- Source particles that may be specified by character descriptors (JSH).

Tallies

- Default dose functions (LSW/JSH);
- Pulse height light tally with anticoincidence: FT8 PHL (GWM);
- Coincidence capture tally and PTRAC file: FT8 CAP (MTS/SJT/DRM/JSH);
- Residual nuclei tally: FT8 RES (JSH);
- Lattice tally speedup (GWM);
- Proton reaction multipliers with FM cards (JSH);
- Photonuclear reaction multipliers with FM cards (JSH/GWM);
- Expanded radiography tally specification (JSH); and
- Cosine bins that may be specified in degrees and for F2 tallies (JSH).

Other Input File Extensions

- Logarithmic interpolation on input cards;
- Auxiliary input files (READ);
- HISTP file size control (HISTP);
- DXTRAN/detector underflow control (DBCN); and
- PTRAC file for coincidence counting (PTRAC).

Graphics

- Enhanced color geometry plots (GWM/JSH);
- 2D color tally contour plots, including lattices and radiography (GWM);
- Geometry plot of weight-window generator superimposed mesh (JSH);
- i,j,k lattice indexing in geometry plots (JSH);
- Photonuclear cross-section plots (JSH);
- Proton and photonuclear cross-section plots (JSH);and
- Pause command for tally and cross-section plots (JSH).

Parallel Processing

- Distributed memory multiprocessing for all particles and energies (GWM);
- Message passing interface (MPI) multiprocessing (JL/GWM); and
- Significant speedup of criticality problems run with MPI (GWM/NAC).

Compiling, configuration, and installation

- FORTRAN90 modularity and dynamic memory allocation (GWM);
- F90 autoconfiguration (TLR/HWE);
- 64-bit integer support (GWM); and
- NAG/IBM/INTEL compiler extensions.

1.2. Guarantee

MCNPX is guaranteed. We are so confident of the quality of MCNPX that we will pay $20 to the first person finding anything that does not meet or exceed the capabilities of MCNPX 2.3.0 and MCNP4C3. We also will pay a brand new $2 bill for any error in MCNPX that has been inherited from its constituent codes.[2]

MCNPX is a better quality code than MCNP4C3. First, it corrects many MCNP4C3 problems. Second, cash awards have been earned less frequently with MCNPX than with MCNP4C3 and its predecessors, and most of those awards are for problems carrying over from older code versions; very few have been put into the new MCNPX versions. A listing of winners is available at http://mcnpx.lanl.gov/. MCNPX bugs are described in the newsletter for each MCNPX version.

1.3. Availability

MCNPX 2.4.0 is available from the RSICC in Oak Ridge, Tennessee, USA, at http://www-rsicc.ornl.gov/. MCNPX 2.4.0 also is available from the OECD NEA Data Bank in Paris, France, at http://www.nea.fr/.

An essential part of the MCNPX software quality assurance plan is the beta test program. Before a code version goes to RSICC or OECD/NEA, it is made available to more than 1000 MCNPX beta testers worldwide. MCNPX 2.5.d is available to beta testers on the MCNPX website at http://mcnpx.lanl.gov/. To apply for a beta test password and to have access to the latest MCNPX versions, contact Laurie Waters at lsw@lanl.gov.

[2] Cash Award Fine Print: Offer is subject to cancellation or modification without notice. A bug is defined as an error in the source code that we choose to correct. We make awards for even the most trivial or insignificant problems but not for proposed code enhancements or proposed extended capabilities. Awards are given only to the first MCNPX user reporting a problem. Reported problems must be reproducible, and awards are paid when the correction is integrated into a forthcoming MCNPX version. We believe that MCNPX and its predecessor codes are the most error-free and robust Monte Carlo radiation transport capabilities, and we back them with a cash guarantee.

All beta test, RSICC, and OECD/NEA versions of MCNPX are guaranteed with cash awards.

2.0. PHYSICS EXTENSIONS

The following physics capability extensions are available and are controlled by the input cards listed in parentheses:

- Mix and match (PHYS:N, PHYS:H, MX);
- Extension of neutron model physics below 20 MeV (PHYS:N, PHYS:H, PHYS:x);
- Fission multiplicity (PHYS:N);
- Light-ion recoil (PHYS:N, PHYS:H);
- Photonuclear model physics (PHYS:P);
- Photon Doppler broadening from MCNP5 (PHYS:P);
- Inline generation of double differential cross sections and residual nuclei (LCA);
- CEM2k physics (LCA);
- INCL4/ABLA physics models (LCA, LEA, LCC); and
- Improved S(α,β) physics (MT).

In the following descriptions of input cards, **bold face type** is used to highlight extensions from earlier MCNP or MCNPX input.

2.1. Neutrons: PHYS:N

PHYS:N *EMAX EAN IUNR DNB* ***TABL FISM RECL***

EMAX = upper energy limit (default = 100 MeV)

Note: EMAX must be higher than the highest energy in the problem or the physics *is wrong.* But setting EMAX too high causes excessively coarse energy binning of model physics, which is inaccurate. For problems with energies above 100 MeV, EMAX should be chosen carefully; the default is appropriate for problems with energies below 100 MeV.

EAN = analog capture below *EAN;* implicit capture above EAN (default = 0 MeV)

IUNR = unresolved resonance range probability table treatment
= 0/1 = on/off (default = 0) when unresolved data are available

DNB = delayed neutrons from fission
-1 = analog production of delayed neutrons from fission (default)
0 = treat prompt and delayed neutrons as prompt
n = biased production: produce up to *n* delayed neutrons per fission ($n > 0$ disallowed in KCODE)

TABL = use data tables below *TABL*; physics models above *TABL*
= -1 (default) (Mix and Match) When tables are available, use them up to their upper limit and use physics models above

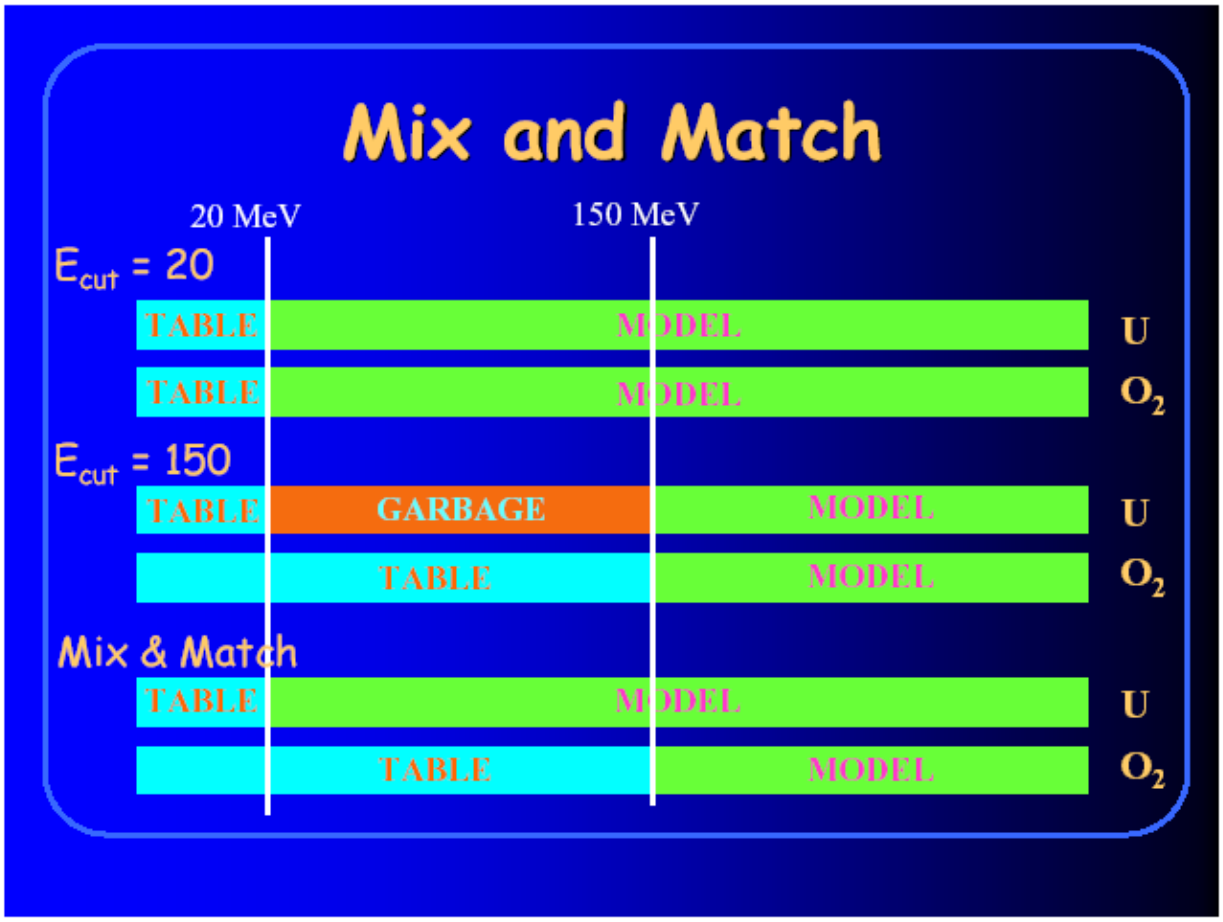
FISM = fission multiplicity
= 0 (default) MCNP treatment. The number of neutrons per fission is the integer above or below ν. If $\nu = 2.7$, then the number of neutrons will be two 30% of the time and three 70% of the time.
= FWHM: sample Gaussian with full-width half-maximum of FWHM about ν
= -1: sample Gaussian with FWHM appropriate for fissioning nuclide (recommended)

RECL = 0 (default) no light-ion recoil
≥ 0: light ion recoil. Produce $0 \leq$ *RECL* $\leq$ 1 light ions (*h*, *d*, *t*, *s*, *a*) at each elastic scatter with light nuclei (H, D, T, ^{3}He, ^{4}He). The ionization potential is accounted for, and the proper two-body kinematics is used (with neutron free-gas thermal treatment if appropriate) to bank the created particles with the proper energy and angle. *MODE n h d t s a . . .* is required to produce 1 light ions (*h*, *d*, *t*, *s*, *a*). *CUT:x 2J 0* for *x* = *h*, *d*, *t*, *s*, *a* is recommended so that the low-energy recoil ions produced are not killed by energy cutoff.

2.1.1. Mix and Match (TABL)

The *TABL* entry on the PHYS:N and PHYS:H cards controls mix and match. If the energy, *E*, is greater than *TABL,* physics models will be used above *E* = *TABL*. It now is possible to use physics models below 20 MeV. If *tabl* = -1, then mix and match is used and the data tables are used for their full energy range, when available, for each nuclide, even if other nuclides in the problem do not have data tables available in that energy range.

The MCNPX mix-and match-capability is illustrated as follows:



Two nuclides are present in this example: oxygen and uranium. The oxygen data table goes from 0–150 MeV; the uranium data table goes from 0–20 MeV. If *TABL* = 20, then nuclear data tables are used below 20 MeV and physics models above; the superior table data for oxygen between 20–150 MeV is ignored. If *TABL* = 150, then nuclear data tables are used below 150 MeV and physics models above; the values for uranium at 20 MeV are used (incorrectly) in the range 20–150 MeV. But if *TABL* = -1 (default), mix and match is used: both oxygen and uranium use the table data where it exists and physics models above the maximum energy.

See the discussion under mix and match for the MX card, below.

2.1.2. Fission Multiplicity (FISM)

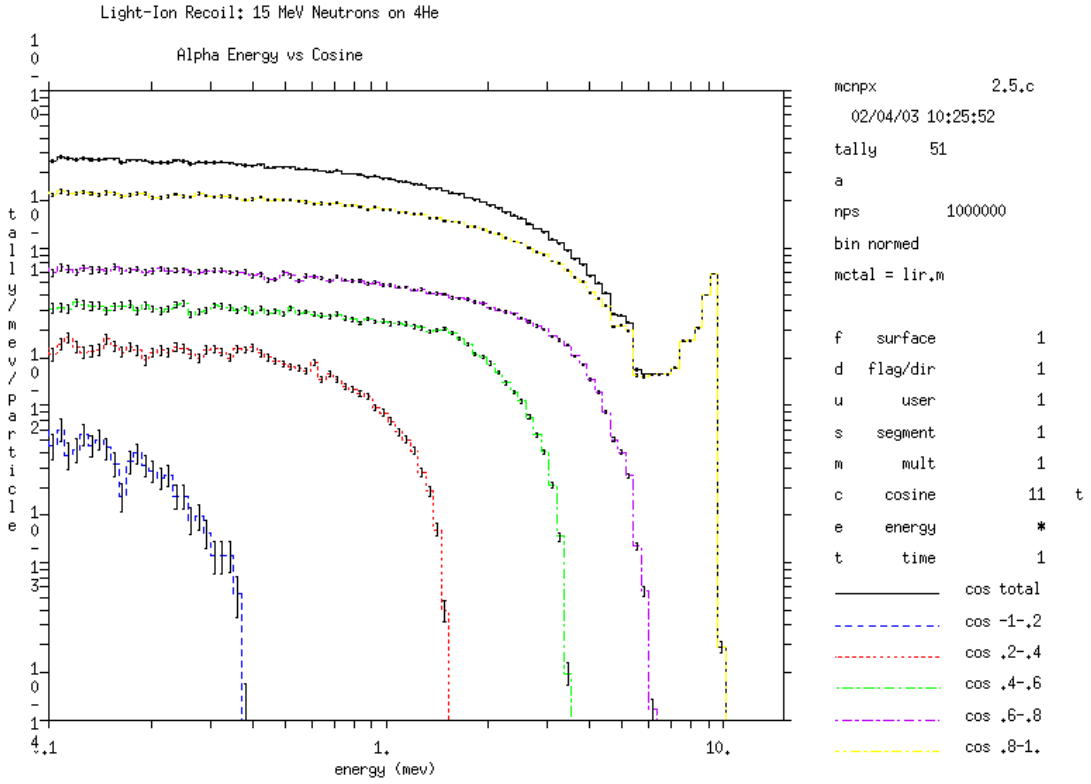
Fission multiplicity is the number of neutrons produced in a fission. The nuclear data tables provide the average number fission neutrons, ν, per fission. The default MCNPX treatment is the MCNP treatment: the number of neutrons per fission is the integer above or below ν. If $\nu = 2.7$, then the number of neutrons will be two 30% of the time and three 70% of the time. If the sixth entry, *FISM,* on the PHYS;N card is positive, then ν is sampled from a Gaussian with FWHM = *FISM*. If *FISM* < 1, then ν is sampled from a Gaussian with FWHM = 1.079, unless the fissioning nuclide is one of the following:

Nuclide	FWHM
92233	1.041
92235	1.072
92238	1.230
94236	1.110
94238	1.115
94239	1.140
94240	1.109
94242	1.069
96242	1.053
96244	1.036
98252	1.207

2.1.3. Light-Ion Recoil (RECL)

MCNPX can produce and track ions created by elastic recoil from neutrons or protons. Neutrons and protons undergoing elastic scatter with light nuclei (H, D, T, ^{3}He, and ^{4}He) can create ions (protons, deuterons, tritons, ^{3}He, and α) that are banked for subsequent transport.

The following picture shows the energy-angle production of alphas created from 15-MeV neutrons striking ^{4}He. Note that in the forward bin, cosine $.8 < \mu < 1$, the α energy goes up to the theoretical maximum of 10 MeV.



The input file for this example is as follows:

```
Test of light ion recoil
1  1 1e-5 -1
2  0       1

1 so 1.e-5

mode n a
imp:n,a 1 0
phys:n 6j 1
sdef erg=15
print -161 -162
tmp1 1e-20 0
fcl:n 1 0
m1 2004 .2
cut:a j 0
nps 1000000
f51:a 1
e51 .1 100log 20
c51 -.8 8i 1 t
fq51 e c
```

The plot commands are in the following plot command file:

```
rmct lir.m tal 51 xlim .1 15 loglog &
title 1 "Light-Ion Recoil: 15 MeV Neutrons on 4He" &
title 2 "Alpha Energy vs Cosine" &
fix c 11 label 1 "cos total" cop fix c 6 label 2 "cos -1-.2" &
cop fix c 7 label 3 "cos .2-.4" cop fix c 8 label 4 "cos .4-.6" &
cop fix c 9 label 5 "cos .6-.8" cop fix c 10 label 6 "cos .8-1."
```

2.2. Photons: PHYS:P

PHYS:P *EMCPF* *IDES* *NOCOH* *ISPN* ***NODOP*** ,

where:

EMCPF	= upper energy for detailed physics (default = 1 MeV)
IDES	= generate electrons by mode E or thick-target-bremsstrahlung (default = 0 = on)
NOCOH	= coherent (Thomson) scattering (default = 0 = on)
ISPN	= -1/0/1 = analog/off/biased. The bias causes a photonuclear event at each photoatomic event. (default = 0 = off)
NODOP	= 0/1 = on/off Doppler energy broadening. (default = 1 = off)

2.2.1. Photonuclear Model Physics (ISPN)

Photonuclear physics models enable (γ,*n*) and other photonuclear reactions when photonuclear data tables are unavailable. When some photonuclear data tables are available, MCNPX will mix and match, using tables when available and physics models when no tables are available. There is no change in user interface; the user simply gets the new gdr.dat file from the MCNPX source file, src/DATA/CEM/gdr.dat.

The MCNPX photonuclear physics model modifications adjust the photofission cross sections in CEM by the ratio of fission and neutron evaporation-level density parameters (*wam*). For selected isotopes (implemented for ^{235}U and ^{232}Th), a list of energy-dependent *wam* parameters was generated matching the fissility of the BOFOD photonuclear cross-section data. The lists are entered into the code as data statements in the newly created subroutine set_*wam*. *F* provides a '*wam*' parameter for a requested nuclide 'IZA' at an incident photon energy of 't0mev' interpolating between two tabulated values. If data for a requested nuclide are not available, *wam* is returned as 0.0. We hope to provide *wam* parameters for more isotopes in the future.

Photonuclear models are designed to work with the CEM2k physics package and are fragile or may not work with other packages.

2.2.2. Photon Doppler Broadening (NODOP)

The MCNP5 photon Doppler broadening capability[3] developed by Avneet Sood is now available in MCNPX. Unlike MCNP5, the default is "off" (PHYS:P 4j 1) because the effect is small but time consuming. When photon Doppler broadening is turned on (NODOP = 0), it has no effect unless photon Doppler broadening momentum profile data are available in the photon library. These data are available in the MCPLIB03 and MCPLIB04 photon libraries with ZAID identifiers .03p and .04p.

The electron binding effect on a scattered photon's energy distribution appears as a broadening of the energy spectrum due to the precollision momentum of the electron. The effect applies to incoherent scatter (Compton scatter). The scattered energy of a Doppler-broadened photon is calculated by selecting an orbital shell, sampling the projected momentum from the Compton profile, and then calculating the scattered photon energy.

Two research notes on photon Doppler broadening are available on the MCNPX web site, http://mcnpx.lanl.gov/documents/. The following is quoted from one of these research notes (X-5:AS-02-16):

> Incoherent scattering of an incident photon can occur with a bound electron in a shell of a material and will generate a Compton electron and a scattered photon. The electron binding effects become important when the incident photon energy is near a few hundred keV. The result of the binding effects on the angle and energy of the scattered photon must be taken into account for accurate simulation of low-energy photon transport. The effect of the bound electron on the scattered photon's angular distribution appears as a reduction in the total scattering cross section in the forward direction. MCNP currently accounts for the electron binding effects on the angular distribution of the scattered photon by modifying the Klein-Nishina differential cross section with a form factor. The electron binding effect on the scattered photon's energy distribution appears as a broadening of the energy spectrum due to the precollision momentum of the electron. This effect on the energy distribution of the incoherently scattered photon is called Doppler broadening.

2.3. Protons: PHYS:H

PHYS:H *EMAX EAN* ***TABL J ISTRG J RECL***

EMAX = upper energy limit (default = 100 MeV)
Note: EMAX must be higher than the highest energy in the problem or the physics *is wrong.* But setting EMAX too high causes excessively coarse energy binning of model physics which is inaccurate. For problems with energies above 100 MeV, EMAX should be carefully chosen; the default is fine for problems with energies below 100 MeV.

EAN = analog capture below *EAN;* implicit capture above EAN (default = 0 MeV)

[3] X-5 Monte Carlo Team, "MCNP—A General Monte Carlo N-Particle Transport Code, Version 5, Volume II: User's Guide," Los Alamos National Laboratory report LA-CP-03-0245 (April 24, 2003), pp. 2–59.

TABL = use data tables below *TABL*; physics models above *TABL*
= -1 (default) (Mix and Match). If tables are available, use them up to the upper energy limit and use physics models above.

J = jump (unused)

ISTRG = charged particle straggling control
= 0 Vavilov (default, best)
= 1 Continuous slowing down approximation
= -1 old MCNPX 2.2.4 method

J = jump (unused)

RECL = light ion recoil. Produce 0 < *RECL* < 1 light ions (*h*, *d*, *t*, *s*, *a*) at each elastic scatter with light nuclei (H, D, T, ^{3}He, ^{4}He). The ionization potential is accounted for, and the proper two-body kinematics is used to bank the created particles with the proper energy and angle. MODE h d t s a … is required to produce light ions (h, d, t, s, a). *CUT:x 2J 0* for x = h, d, t, s, a is recommended so that the low-energy recoil ions produced are not killed by energy cutoff. Note that protons colliding with hydrogen to produce more protons can produce an overwhelming number of protons; caution is required and *RECL < 1* may be needed.

See the definitions of *TABL* and *RECL* in the description of the neutron physics card, PHYS:N, above.

2.4. Charged Particles: PHYS:x

PHYS:x *EMAX 3J* ***ISTRG***

EMAX = upper energy limit (default = 100 MeV)

Note: EMAX must be higher than the highest energy in the problem or the physics *is wrong*. But setting EMAX too high causes excessively coarse energy binning of model physics which is inaccurate. For problems with energies above 100 MeV, EMAX should be carefully chosen; the default is fine for problems with energies below 100 MeV.

J = jump (unused)

ISTRG = charged particle straggling control
= 0 Vavilov or Prael's new straggling model, which is an energy correction addressing stopping powers. (default, best)
= 1 Continuous slowing down ionization model
= -1 old MCNPX 2.2.4 method

2.5. Mix-and-Match Nuclide Replacement: MX

The **MX** card enables materials substitution for different particle types. It is an extension of, and replacement for, the MPN card for photonuclear data:

MXn:p *zaid1 zaid2 ...*

where n = material number of an Mn card that MUST precede the MXn card;
p = particle type (n, p, h)

zaidn = ZA of replacement nuclide for the nth nuclide on the Mn card.

Only particle types n (neutron), p (photonuclear), and h (proton) are allowed on the MX card. No substitutions are allowed for photoatomic (p) and electron (e) data because those data sets are complete. The MXn:P card is an exact replacement of the MPNn card and specified photonuclear nuclide substitutions (library type u). zaidn = 0 is allowed on MXn:P (photonuclear substitution) to specify no photonuclear data for a specific photoatomic reaction. zaidn = model is allowed on the MXn:N and MXn:H (neutron and proton substitution) to allow models to be mixed with tabular data. As an example, consider the following input file:

```
mode n h p
m1          1002 1      1003.6 1    6012 1      20040  1        nlib .24c
mx1:n       j           model       6000        20000
mx1:h       model       1001        j           j
mpn1        6012        0           j           j
```

MCNPX will issue the following warnings:

```
warning. MPNn will soon be obsolete. use MXn:p instead.
warning. photonuclear za = 6012 different from nuclear za = 1002
warning. photonuclear za =    0 different from nuclear za = 1003
```

Note that models will be used for neutron tritium and proton deuterium. The MPN card still works but has a warning. The mixing and matching is summarized in Print Table 101:

1particles and energy limits print table 101

particle type			particle cutoff energy	maximum particle energy	smallest table maximum	largest table maximum	always use table below	always use model above
1	n	neutron	0.0000E+00	1.0000E+37	1.5000E+02	1.5000E+02	0.0000E+00	1.5000E+02
2	p	photon	1.0000E-03	1.0000E+02	1.0000E+05	1.0000E+05	1.0000E+05	1.0000E+05
9	h	proton	1.0000E+00	1.0000E+02	1.5000E+02	1.5000E+02	0.0000E+00	1.5000E+02

The MCNPX mix-and-match capability[4] enables mixing and matching physics models and data tables. It is now possible to specify some nuclides with models and other nuclides with data tables (isotope 'mixing'). It is also possible to use data tables up to their maximum energy value and then use models above that energy, even when the maximum table energy differs from nuclide to nuclide ('energy matching') [8].

As an example, consider protons interacting with a Bismuth Germinate particle detector (BGO). Because the present LA-150 nuclear data libraries [9] do not include Germanium, it was previously possible to use only physics models for all nuclides in the entire problem. With the

[4] John S. Hendricks, "MCNPX Model/Table Comparison," Los Alamos National Laboratory Report, LA-14030 (March 2003)

mix-and-match capability, Bismuth and Oxygen can be modeled with the more accurate nuclear data tables, whereas Germanium utilizes a physics model.

As another example, consider a neutron problem with Deuterium and Tritium. The available Deuterium library goes up to 150 MeV, but the Tritium library goes up to only 20 MeV. Previously, either neutron physics models above 20 MeV (neglecting the Deuterium table data up to 150 MeV) or nuclear data tables below 150 MeV (using the 20-MeV Tritium data throughout the entire 20-MeV to 150-MeV range) had to be used. With the mix-and-match capability, Deuterium uses tables up to 150 MeV and uses physics models above 150 MeV; Tritium uses data tables up to 20 MeV and uses physics models above 20 MeV.

Figure 1 shows an example of the energy matching capability. 100 MeV neutrons are incident on a 8.433 cm long, 3.932 cm radius BGO crystal. The crystal contains 21% Bi, 16% Ge and 63% O. No Ge libraries are currently available. The solid line represents flux in the crystal with the full mix-and-match capability, which uses all libraries up to their energy limits, and physics models above those limits and for Ge. The dashed line calculation uses the old method of substituting Arsenic for the missing Ge library, using the libraries up to 20 MeV, and using physics models above. The dotted line uses Bi and O libraries up to their limits of 150 MeV; the As library is used up to its limit of 20 MeV, and then the 20 MeV data is used from 20-150 MeV; above 150 MeV physics models are used for all three nuclides. This last option is least desirable, but was often used in past code versions to take advantage of the 150 MeV libraries, even though many data libraries only go to 20 MeV.

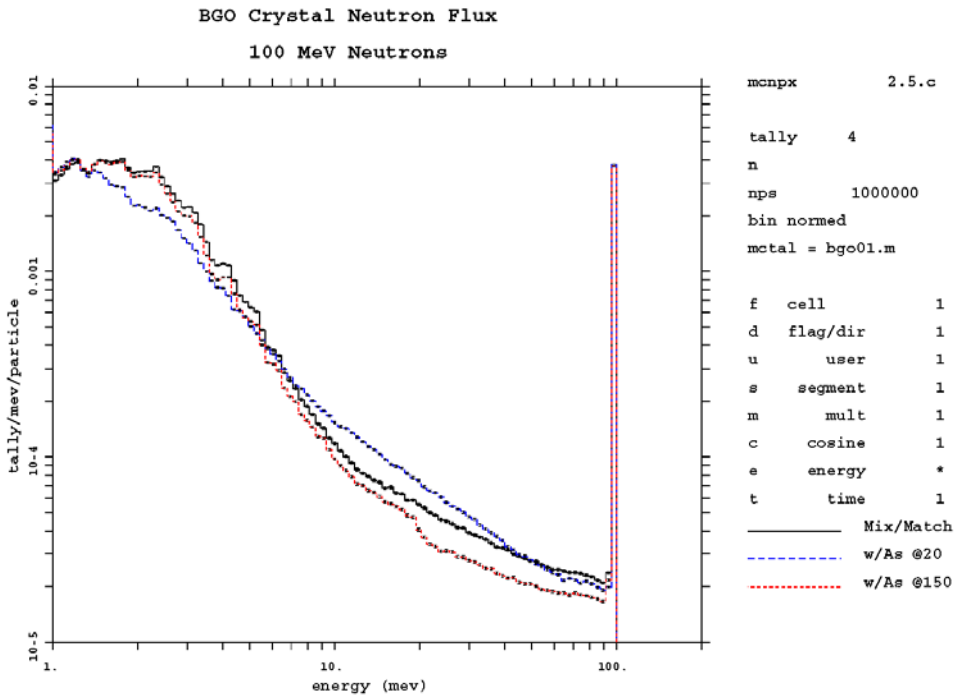


Fig. 1. Comparison of different Germanium library and model options.

The mix-and-match capability is particularly useful for photonuclear calculations because few photonuclear data tables are currently available. Now libraries are used when available and models are used otherwise. Note that photonuclear physics is modeled with the new CEM2k model, regardless of whether CEM is used for other particles.

It is also possible now to substitute different nuclides for different particle types. For example, natural Carbon and Calcium can be used for neutrons whereas ^{12}C and ^{40}Ca can be used for protons and photonuclear reactions.

2.6. Physics Models: LCA

LCA *IELAS IPREQ IEXISA ICHOIC JCOUL NEXITE NPIDK* ***NOACT ICEM***

IELAS = 0 / 1 / 2 (default) = no / neutron only / neutron and proton elastic scattering
IPREQ = 0 = no pre-equilibrium model will be used
= 1 (default) = use pre-equilibrium model after intranuclear cascade
= 2 = select IPREQ = 1 and IPREQ = 3 randomly if IEXISA = 0
= 3 = use pre-equilibrium model instead of the intranuclear cascade if IEXISA = 0
IEXISA = 0 = do not use ISABEL intranuclear cascade (default if ICEM = 2 = INCL4)
= 1 (default) = use Bertini for nucleons and pions and ISABEL for other particles
= 2 = use ISABEL for all particles
ICHOIC = ISABEL model control (0023 = default)
JCOUL = 0 / 1 (default) = no / yes Coulomb barrier for incident charged particles
NEXITE = 1 (default) / 2 = subtract nuclear recoil energy to get excitation energy
NPIDK = 0 (default) / 1 = force pi- nuclear capture below pi- energy cutoff
NOACT = -2 = source particles immediately collide; all progeny escape. Used to compute double differential cross sections and residual nuclei.
= -1 = nuclear interactions of source particles only – transport and slowing down are off. Used to compute double-differential cross sections with XSEX code.
= 0 = turn off all nonelastic reactions
= 1(default) = normal transport
= 2 = attenuation mode – transport primary source particles without nonelastic
ICEM = 0 (default) = Use Bertini or ISABEL model determined by IEXISA
= 1 = use CEM2k model
= 2 = use INCL4 model (default ABLA fission-evaporation)

2.6.1. Inline Generation of Double Differential Cross Sections and Residual Nuclei

The *NOACT* option on the LCA card enables MCNPX to calculate a single interaction in the physics model region. If the eighth entry on the LCA card is –2,

LCA 7J **–2**

then the source particle immediately will have a collision, and all subsequent particles will escape. That is, LCA(8) = –2 causes the source particle to have a distance-to-collision of zero, and all subsequent tracks have a distance-to-collision of infinity.

The double differential cross sections and distributions of residual nuclei for a single nuclear interaction thus may be calculated directly in MCNPX. Tallying of the residual nuclei is dicussed

later in the FT8 RES tally description. Tallying of the differential cross section can be done with standard F1 surface tallies as shown in the following example. The input file models a 1.2-GeV proton source having a single collision with ^{208}Pb.

```
Test of p(1.2GeV)+Pb(208)
1 1 -11. -1 imp:h 1
2 0        1 imp:h 0

1 so .01

mode h n
sdef par h erg=1200 vec 0 0 1 dir 1
m1 82208 1
phys:h 1300 j 0
phys:n 1300 3j 0
nps 10000
fc1  *** neutron angle spectra tally ***
f1:n  1
ft1  frv 0 0 1
fq1 e c
*c1 167.5 9i 17.5 0 T
e1 1 50log 1300 T
lca   2 1 1 23 1 1 0 -2 0
```

The differential cross section for neutron production is tallied in the F1 current tally with energy and time bins. This tally is simply the neutrons that are created from the single proton collision with lead and then escape. These data may be plotted with MCNPX using the tally plotter and the following execute line command:

MCNPX Z

where the command file, COM91, is

```
rmctal=mctl91
file all loglog xlim 1 1300 ylim 1e-6 1 &
fix c 13 cop fix c 1 cop fix c 6 cop fix c 12
```

In Fig. 3, the first line (solid black) is the energy spectrum over all angles, the second (blue dashed) is the 180^{o} output, the third (red dotted) is the 90^{o} output, and the fourth (green broken) is the 0^{o} output.

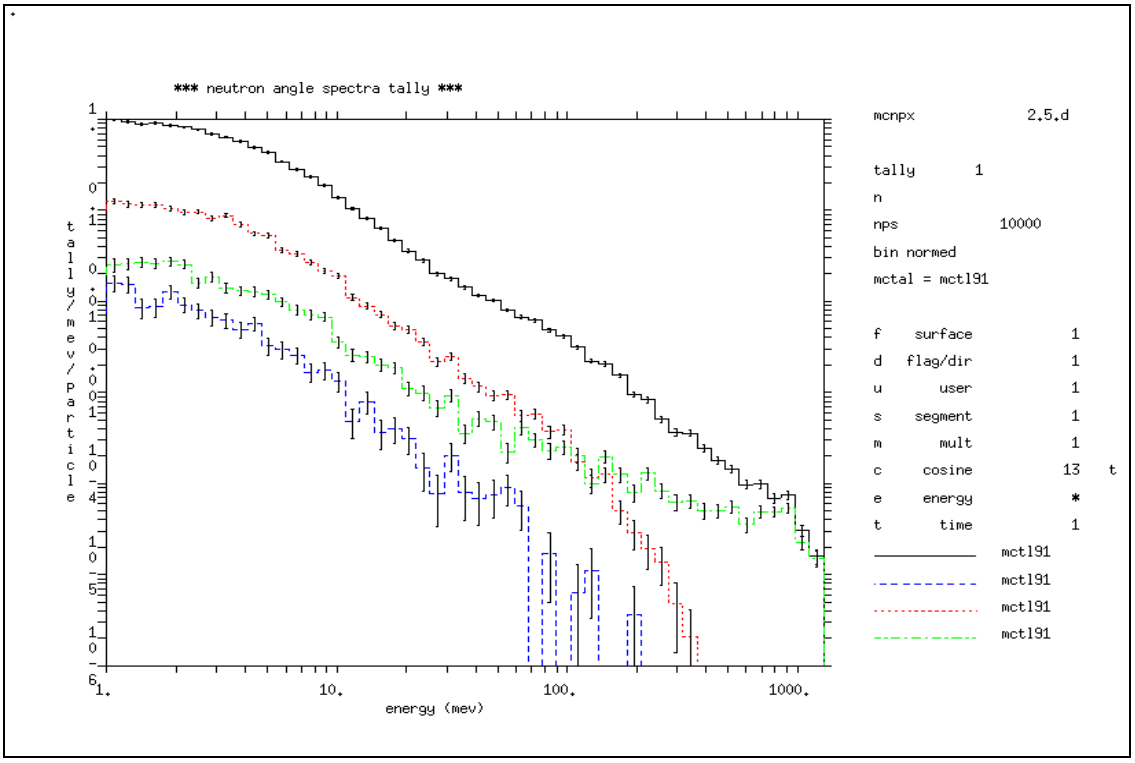


Fig. 3. Differential cross sections at all angles, 180°, 90°, and 0° for 1.3-GeV protons on $^{208}_{82}$Pb.

2.6.2. CEM2k Physics Model (ICEM)

The MCNPX CEM physics model has been upgraded from CEM95 to CEM2k[5] It is still controlled solely by the 9th entry, ICEM, on the LCA card. The model assumes that reactions occur in three stages. The first stage is the Intra Nuclear Cascade (INC), in which primary particles can be re-scattered and produce secondary particles several times before absorption by or escape from the nucleus. The excited residual nucleus remaining after the cascade determines the particle-hole configuration that is the starting point for the pre-equilibrium stage of the reaction. The subsequent relaxation of the nuclear excitation is treated in terms of an improved Modified Exciton Model of pre-equilibrium decay followed by the equilibrium evaporative final stage of the reaction, which is competing with the fission and Fermi-breakup channels.

CEM2k incorporates new approximations for the elementary cross sections used in the cascade, using more precise values for nuclear masses and pairing energies, corrected systematics for the level-density parameters, and several other refinements. Improved algorithms decrease the computing time by up to a factor of six for heavy targets. Other improvements were motivated by new measured data on isotope production from GSI experiments. CEM2k has a longer cascade state, less preequilibrium emission, and less evaporation from more highly excited compound nuclei as compared with earlier versions. CEM2k also has better models of

[5] S. G. MASHNIK, A. J. SIERK, "Recent Developments of the Cascade-Exciton Model of Nuclear Reactions," *Los Alamos National Laboratory report* LA-UR-01-5390, and International Conference on Nuclear Data for Science and Technology, Tsukuba, Japan (October 7–12, 2001).

neutron, radionuclide, and gas production in accelerator-transmutation-of-waste spallation targets.

A photonuclear physics package has been added to CEM2k by Franz Gallmeier (ORNL) for photon energies from 8 MeV to about 2 GeV, and includes the Giant Dipole and Quasi-Deuteron resonances. These photonuclear physics models compliment existing photonuclear data evaluations in that they may be used for nuclides where no tabular data exist. Also, they may be used for tabular-data nuclides above the 150-MeV upper-energy boundary of the tables.

2.6.3. INCL4/ABLA (Cugnon/Schmidt) Physics Models (ICEM)

The IntraNuclear Cascade Liege (INCL4) and ABLA fission-evaporation models are now available in MCNPX. They are controlled by the LCA, LCC, and LEA input cards:

LCA(9) = **2** INCL4 model (sets LCA(3) =*IEXISA = 0)*
LEA(7) = **2** ABLA fission evaporation
LCC = control parameters for INCL4

INCL4 and ABLA may be used in various combinations with other physics models:

Bertini/Dresner:	LCA 2 1 1 23 1 1 0 1 0	$ MCNPX Default: Bertini
	LEA 1 4 1 0 1 0 0 1	$ MCNPX Default: Dresner
CEM2k	LCA 8J 1	$ CEM2k works alone
ISABEL/Dresner	LCA 2J 2	$ ISABEL
Bertini/ABLA	LEA 6J 2	$ ABLA
ISABEL/ABLA	LCA 2J 2	$ ISABEL
	LEA 6J 2	$ ABLA
INCL4/Dresner	LCA 8J 2	$ INCL4
INCL4/ABLA	LCA 8J 2	$ INCL4
	LEA 6J 2	$ ABLA

These combinations also may be shown in the following table:

	LCA(3) *IEXISA*	LCA(9) *ICEM*	LEA(7) *IEVAP*
Bertini/Dresner	1	0	0
ISABEL/Dresner	2	0	0
Bertini/ABLA	1	0	2
ISABEL/ABLA	2	0	2
CEM2k	-	1	-
INCL4/Dresner	0	2	0
INCL4/ABLA	0	2	2

The INCL4 model is based largely on the work of Joseph Cugnon at the University of Liege in Liege, Belgium. It generally is coupled with the ABLA fission-evaporation model that was developed principally by Karl-Heinz Schmidt at Gesellschaft für Schwerionenforschung, mbH, Darmstadt, Germany. Its integration into MCNPX has been done principally by Jean-Christophe David at Commissariat à l'Energie Atomique-Saclay, France.

INCL4 and ABLA are intended for use in the 200-MeV to 2-GeV energy range. There are only two free parameters in INCL4: the potential depth V_0 (default = 45 MeV) and the overall factor f_{stop} (default = 1.0). These are controlled by the LCC card.

Note that the INCL4 model, in its present implementation, is much slower than the Bertini and CEM2k models.

2.7. INCL4 Options: LCC

LCC ***STINCL V0INCL XFOISAINCL NPAULINCL NOSURFINCL***

The LCC card specifies options for the INCL4 (IntraNuclear Cascade, Liege) model and ABLA fission-evaporation model. INCL is invoked by setting the 9th LCA card entry to 2 and ABLA is invoked by setting the 7th LEA card entry, IEVAP, to 2. The LCC card entries are:

(1)	*STINCL*	rescaling factor of the cascade duration (default = 1)
(2)	*V0INCL*	potential depth (default = 45 MeV)
(3)	*XFOISAINCL*	factor X_f to control the WS potential extension from R_o. $R_{max} = R_o + X_f * A$ where A = diffusiveness (default = 8)
(4)	*NPAULINCL*	Pauli principal flag = 1 strict = 0 statistical (default) = 2 no
(5)	*NOSURFINCL*	nuclear surface flag = 1 strict – sharp surface = 0 diffuse – with WS density, time without b dependence = -1 diffuse – with WS density, time with B dependence = -2 diffuse – with WS density and INCL4 stopping time (default)

2.8. ABLA Fission-Evaporation Model: LEA

LEA *IPHT ICC NOBALC NOBALE IFBRK ILVDEN* ***IEVAP*** *NOFIS*

IPHT = 0 / 1 (default) = no / yes generate de-excitation photons
ICC = 0 / 1 / 2 / 3 / 4 (default) = continuum / Troubetzkoy / intermediate / spin-dependent / full PHT physics model.
NOBALC = 0 / 1 (default) no / yes – turn off mass-energy balancing in cascade
NOBALE = 0 (default) / 1 = mass-energy balancing in evaporation
IFBRK = 0 / 1 (default) = Fermi breakup model nuclide range
ILVDEN = -1 / 0 (default) / 1 = HETC / Gilbert / Julich – level density model
IEVAP = 0 (default) / 1 / 2 = RAL / ORNL / ABLA fission-evaporation model
NOFIS = 0 / 1 (default) = suppress / allow - fission

2.9. Improved S(α,β) Treatment: MT

The S(α,β) thermal neutron treatment user interface is unchanged, but the underlying secondary energy treatment is improved. The S(α,β) thermal neutron treatment in many cases uses discrete energies instead of 32-equiprobable bin histogram energies. The result is nonphysical spikes in the thermal neutron spectrum. These are now smoothed out by an algorithm provided by Bob Little and Eric Pitcher. MCNPX can still track the old algorithm by setting DBCN(21) = 1.

3.0. SOURCE FEATURES

Most MCNPX source extensions are controlled by the SDEF card:

- Source particles that may be specified by descriptors;
- Positron sources;
- Spontaneous fission;
- Multiple source particle types;
- Sources on cylindrical surfaces;
- Repeated structures source-paths.

3.1. Particle-Type Specification: SDEF

The source particle type now may be specified on the SDEF card by either its symbol

SDEF PAR = **h**

or by its number.

SDEF PAR = 9

3.2. Positron Sources: SDEF

Positron sources may now be specified as

SDEF PAR = **-e**
or SDEF PAR = **-3** .

Note that positron physics in MCNPX, just as with MCNP and the Integrated Tiger Series (ITS), is identical to electron physics except for positron annihilation. Electrons below the energy cutoff are terminated, whereas positrons below the energy cutoff produce annihilation photons. Also, the positrons have a positive charge and may be tallied using the FT card ELC option.

3.3. Spontaneous Fission Sources: SDEF

The spontaneous fission source can be specified in either of two ways:

SDEF par = **SF** normalize summary and tally information by the number of spontaneous fission neutrons; or

SDEF par = **–SF** normalize summary and tally information by the number of histories (generally fission neutrons).

3.3.1. Spontaneous Fission Physics

Eighteen nuclides are available: ^{232}Th, ^{232}U, ^{233}U, ^{234}U, ^{235}U, ^{236}U, ^{238}U, ^{237}Np, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{241}Am, ^{242}Cm, ^{244}Cm, ^{249}Bk, and ^{252}Cf.

Cells are sampled according to the usual SI and SP distributions. If more than one spontaneous fission nuclide is in a source cell, the fissioning nuclide will be chosen proportionately to the product of its atom fraction and the spontaneous fission yield for each nuclide. If no spontaneous fission nuclide is found in a specified source cell, the code exits with a bad trouble error, "spontaneous fission impossible."

The number of spontaneous fission neutrons is then sampled. The spontaneous fission multiplicity data of Ensslin is used. The energies are sampled from a Watt spectrum with appropriate spontaneous fission parameters for the selected nuclide. Currently, only the first spontaneous fission neutron from each history is printed. If the spontaneous fission samples a multiplicity of zero—that is, no neutrons for a given spontaneous fission—then the history is omitted from the first 50 history lists of Print Table 110. The number of source particles is the number of spontaneous fission neutrons, which will be ν times the requested number of source histories on the NPS card.

Fission multiplicity for induced fissions (6h entry, PHYS:N card) automatically is turned on with the default width (FISM = -1 = nuclide dependent). If FISM > 0 on the PHYS:N card, then that value will be used.

3.3.2. Normalization of Summary and Tally Information

The MCNPX spontaneous fission source is different from most other SDEF fixed sources. Let

N = NPS from the NPS card = the number of source particle histories,
W = the average source particle weight, and
ν = the average number of spontaneous fission neutrons per fission.

For most other MCNPX fixed source (SDEF) problems,

summary table source tracks = N,
summary table source weight = W, and
summary tables and tallies are normalized by N.

For the spontaneous fission source, SDEF par = SF ,

summary table source tracks = $\nu \cdot N$,
summary table source weight = W,
summary tables and tallies are normalized by $\nu \cdot N$.

For the spontaneous fission source, SDEF par = –SF,

summary table source tracks = ν·N,
summary table source weight = ν·W,
summary tables and tallies are normalized by N.

3.3.3. Fission Multiplicity Output

Multiplicity and moments are printed in Print Table 117 for both spontaneous and spontaneous plus induced fissions.

```
spontaneous fission source multiplicity and moments.                    print table 117

       ------ by number -----------  ---------------- by weight ----------------------
              fission  multiplicity                    fission   multiplicity
      fissions neutrons    fraction      fissions      neutrons      fraction    error

nu =  0    697      0   6.97000E-02   3.24005E-02   0.00000E+00   6.97000E-02   0.0373
nu =  1   2295   2295   2.29500E-01   1.06685E-01   1.06685E-01   2.29500E-01   0.0197
nu =  2   3261   6522   3.26100E-01   1.51590E-01   3.03180E-01   3.26100E-01   0.0161
nu =  3   2518   7554   2.51800E-01   1.17051E-01   3.51153E-01   2.51800E-01   0.0187
nu =  4   1025   4100   1.02500E-01   4.76478E-02   1.90591E-01   1.02500E-01   0.0305
nu =  5    183    915   1.83000E-02   8.50688E-03   4.25344E-02   1.83000E-02   0.0736
nu =  6     21    126   2.10000E-03   9.76199E-04   5.85720E-03   2.10000E-03   0.2181

  total  10000  21512   1.00000E+00   4.64857E-01   1.00000E+00   1.00000E+00   0.0073


  factorial moments            by number               by weight

          nu                2.15120E+00 0.0054      2.15120E+00 0.0054
      nu(nu-1)/2!           1.91100E+00 0.0116      1.91100E+00 0.0116
   nu(nu-1)(nu-2)/3!        8.86800E-01 0.0219      8.86800E-01 0.0219
nu(nu-1) .... (nu-3)/4!     2.25500E-01 0.0439      2.25500E-01 0.0439
nu(nu-1) .... (nu-4)/5!     3.09000E-02 0.0987      3.09000E-02 0.0987
nu(nu-1) .... (nu-5)/6!     2.10000E-03 0.2180      2.10000E-03 0.2180


spontaneous and induced fission multiplicity and moments.               print table 117

       ------ by number -----------  ---------------- by weight ----------------------
              fission  multiplicity                    fission   multiplicity
      fissions neutrons    fraction      fissions      neutrons      fraction    error

nu =  0    700      0   6.90949E-02   3.25400E-02   0.00000E+00   6.90949E-02   0.0372
nu =  1   2301   2301   2.27125E-01   1.06964E-01   1.06964E-01   2.27125E-01   0.0197
nu =  2   3286   6572   3.24351E-01   1.52752E-01   3.05504E-01   3.24351E-01   0.0161
nu =  3   2558   7674   2.52492E-01   1.18910E-01   3.56731E-01   2.52492E-01   0.0186
nu =  4   1059   4236   1.04531E-01   4.92283E-02   1.96913E-01   1.04531E-01   0.0300
nu =  5    205   1025   2.02349E-02   9.52956E-03   4.76478E-02   2.02349E-02   0.0695
nu =  6     22    132   2.17155E-03   1.02269E-03   6.13611E-03   2.17155E-03   0.2131

  total  10131  21940   1.00000E+00   4.70946E-01   1.01990E+00   1.00000E+00   0.0072


   factorial moments            by number               by weight

          nu                2.16563E+00 0.0054      2.16563E+00 0.0054
      nu(nu-1)/2!           1.94393E+00 0.0115      1.94393E+00 0.0115
   nu(nu-1)(nu-2)/3!        9.16395E-01 0.0216      9.16395E-01 0.0216
nu(nu-1) .... (nu-3)/4!     2.38279E-01 0.0426      2.38279E-01 0.0426
nu(nu-1) .... (nu-4)/5!     3.32642E-02 0.0932      3.32642E-02 0.0932
nu(nu-1) .... (nu-5)/6!     2.17155E-03 0.2130      2.17155E-03 0.2130
```

In the above problem there were 10000 source histories. All were spontaneous fissions. There were 21512 spontaneous fission neutrons produced. The number of source particles and the

source weight listed in the problem summary table for neutrons is also 21512 and 2.1512E+00. Also, from the problem summary table for neutrons there were 131 induced fissions producing 428 fission neutrons.

In the second Print Table 117 there are 10000 + 131 = 10131 fissions. There are 21512 + 428 = 21940 fission neutrons. For nu = 0 the multiplicity fraction is 700 / 10131 = .0690949. The total multiplicity fraction always sums to one. By weight fissions sum to
10131 / 21512 = .470946. By weight fission neutrons sum to 21940 / 21512 = 1.01990.
The by weight multiplicity fractions are the same as the by number multiplicity fractions because analog capture is used in this problem and the entire source is spontaneous fission.

If SDEF PAR = -SF is used, the normalization for tallies, summary information, and some entries in Print Table 117 is by source history. By weight fissions is 10131 / 10000 = 1.01310 instead of .470946. By weight fission neutrons is 2.19400 instead of 1.01990. The by weight multiplicity fractions are divided by the total fission weight, 10131.0, to sum to unity.

The first moment is nu = 21940 / 10131 = 2.16563.The 2^{nd} moment is (2x1 / 2! X 3286 + 3x2 / 2! X 2558 + 4x3 / 2! X 1059 + 5x4 / 2! X 205 + 6x5 / 2! X 22) / 10131 = 1.94393.The 3^{rd} moment is (3x2x1/3! x 2558 + 4x3x2 / 3! x 1059 + 5x4x3 / 3! x 205 + 6x5x4 / 3! x 22) / 10131 = .916395.The 4^{th} moment is (4x3x2x1 / 4! x 1059 + 5x4x3x2 / 4! x 205 + 6x5x4x3 / 4! x 22) / 10131 = .238279.The 5^{th} moment is (5x4x3x2x1 / 5! x 205 + 6x5x4x3x2 / 5! x 22) / 10131 = .0332642.The 6^{th} moment is 6x5x4x3x2x1 / 6! x 22 / 10131 = .00217155.

3.4. Multiple Particles on SDEF Card

Multiple-source particle types may be specified in fixed-source problems. PAR on the SDEF card now may be either a distribution or a dependent distribution.

3.4.1. Source Particle Type as the Independent Variable

```
sdef par=d1 pos fpar d2 erg fpar d3
si1 L h n
sp1   2 1
sb1   1 2
ds2 L 0 0 0 15 0 0
ds3 L 2 3
```

The particle types are protons (at 0,0,0, energy 2 MeV) and neutrons (at 15,0,0, energy 3 MeV).

3.4.2. Source Particle Type as a Dependent Variable

```
sdef par=fpos d2 pos=d1 erg fpos d3
si1 L 0 0 0 15 0 0
sp1   2 1
sb1   1 2
ds2 L h n
ds3 L 2 3
```

The source particles are protons and neutrons, depending on the problem source positions. This source tracks the source described in Section 2.3.1 exactly.

3.4.3. Additional Capabilities and Cautions

- The characters L, S, Q, F, and T are reserved as SI card options. L = discrete source variables; S = distribution numbers, etc. If the first entry on the SI card is L, S, Q, F, or T, it will be interpreted as a distribution option. To use source particle types L, S, Q, F, or T, either the corresponding particle numbers (10, 33, 30, 27, or 32) must be used or L, S, Q, F, or T must be used as the second or later particle type. Generally, it is best to specify the discrete source variable option; therefore, L will be the first entry followed by the particle types. A second L will be interpreted correctly as particle type L. For example:

  SI99 L –H N L Q F T S .

- Antiparticles may be designated. For example:

  SI77 L –E N –H .

- Either characters (n, p, e, h, d, s, t, a, etc.) or numbers (1, 2, 3, 9, 31, 32, 33, 34, etc.) may be used. For example:

  SI98 L –H 3 –32 N .

- Spontaneous fission may be used as a particle type. For example:

  SI87 L SF N .

- Particle types may be listed multiple times to give them different energy distributions, angular distributions, etc., in different parts of the problem. For example:

  SI23 L N n 1 n N .

3.4.4. Tally and Summary Table Normalizations

Tallies are normalized by dividing the total source weight by the number of source histories. Note that weight (WGT on the SDEF card) cannot be a source distribution (either independent or dependent). The weight of particles in the summary tables is controlled by the SI, SP, SB, and DS cards for the particle distribution. In the example shown in Section 2.3.1,

```
sdef par=d1 pos fpar d2 erg fpar d3
si1 L h n
sp1   2 1
sb1   1 2
ds2 L 0 0 0 15 0 0
ds3 L 2 3
```

The total source weight is WGT = 1.0 by default. From the SP1 card, the weight of the neutrons that are produced is 0.3333, and the weight of protons that are produced is 0.6667. From the SB1 card, the total number of neutron tracks is 0.6667 × NPS for neutrons and 0.3333 × NPS for protons (where NPS is the number of source histories on the NPS card). The energy per source particle is normalized to the source particle weight for each source particle type. If the particle

type is not a source particle (e.g., photons in the above problem), then the energy per source particle is normalized to the source particle weight of the lowest particle type. In this example, photon source energy would be normalized in the photon creation and loss summary table by 0.3333, the weight of the source neutrons produced.

Fission multiplicity and FT8 CAP capture tallies (Print Tables 117 and 118) "by number" quantities are always normalized by NPS, the number of histories run (NPS card). NPS generally equals the number of fissions, not fission neutrons, plus other source particles. The "by weight" quantities are normalized by NPS for PAR = SF and by fission neutrons (plus other source particle) for PAR = –SF.

Spontaneous fission has two normalizations: PAR = SF and PAR = –SF. For PAR = SF, the normalization is total source weight, WGT, divided by the total neutron source weight: spontaneous fission neutrons plus other source neutrons.

3.5. Sources on Cylindrical Surfaces: SDEF

Cylindrical surface sources now may be specified on the SDEF card. Furthermore, particle directions distributed relative to the cylindrical source normal may be specified. The cylindrical surface can be, but does not have to be, a cell-bounding problem surface. Likewise, a spherical surface source no longer has to be on a cell-bounding problem surface.

In MCNP and earlier MCNPX versions, the only way to specify a cylindrical surface source was to have a degenerate cylindrical volume source (radius = constant) that is not also a problem surface. Particle direction had to be isotropic from the source point.

3.5.1. Examples

The following examples now work, whereas all failed in previous MCNP and MCNPX versions.

Cylindrical problem surface with default cosine distribution relative to surface normal:

```
SDEF  pos = 0 0 0     rad = 1       ext = d1        axs = 1 0 0     sur = 5   .
```

Cylindrical problem surface with specified angle distribution relative to surface normal:

```
SDEF  pos = 0 0 0     rad = 1       ext = d1        axs = 1 0 0     sur = 5   dir = d2   .
```

Cylindrical surface (degenerate volume source) with specified angle distribution relative to surface normal:

```
SDEF  pos = 0 0 0     rad = 1       ext = d1        axs = 1 0 0     dir = d2   .
```

Spherical surface (degenerate volume source) with specified angle distribution relative to surface normal:

```
SDEF  pos = 0 0 0     rad = 1       dir = d2   .
```

3.5.2. Additional Information and Cautions

- If the cylindrical surface is a problem surface, then the surface number must be specified on the SDEF card with the SUR parameter.
- If both DIR and VEC are specified, then particle directions are relative to VEC rather than to the cylindrical surface normal.
- All former capabilities remain the same:
- volume sources have a default isotropic direction;
- particle directions are relative to VEC if VEC is specified;
- only capabilities that formerly were disallowed are different:
- SUR now may be specified on a cylindrical surface, and the default VEC is the surface normal;
- DIR now may be specified without VEC (so that VEC defaults to the surface normal) for spheres and cylinders; and
- the outward normal to cylindrical surfaces now is generated whenever DIR is specified and VEC is not.

3.6. Repeated Structures Source Specifications: SI

The CEL source specification for repeated structures geometries is now consistent with the tally specification. The old MCNP4C specification still works, but the new one is

```
SDEF CEL=d3 POS=0 6 0 EXT=d1 RAD=d2 AXS= 0 1 0
SI3 L (1<10[0 0 0]<11) (1<10[1 0 0]<11) (1<10[2 0 0]<11)
      (1<10[0 1 0]<11) (1<10[1 1 0]<11) (1<10[2 1 0]<11)
```

4.0. TALLY FEATURES

The MCNPX tally extensions provide a wide range of new capabilities. Note that logarithmic interpolation (Section 5.1) is particularly useful for many tally cards. The applicable tally input cards are in parentheses after the features they control.

- Default dose functions (DF);
- Lattice tally speedup (F);
- Radiography tallies: translate new MCNP5 FIP, FIR, and FIC radiography input cards as MCNPX radiography tallies PI, TIR, and TIC;
- Proton and photonuclear reaction multipliers (FM);
- Cosine bins that may be specified in degrees and for F2 tallies (C);
- Pulse height light tally with anticoincidence: FT8 PHL;
- Coincidence capture tally & PTRAC file: FT8 CAP;
- Residual nuclei tally: FT8 RES.
-

4.1. Default Dose Functions (DF)

The DE/DF dose function cards are unchanged but now have extensions. As before, dose conversions may be input as a table. Note that the interpolation int = log or int = lin now may be placed anywhere, and n = tally number, which implies particle type.

DEn E1 E2 int E3 ...
DFn F1 int F2 F3 ...

The dose conversion capability is extended to provide standard default dose functions. These are invoked by omitting the DE card and using keywords on the DF card:

DFn iu=j fac=F int ic=I ,

where the following entries are all optional:

iu = 1 = US units (rem/h)
iu = 2 = international units (sieverts/h)
Default: iu = 2 international units (sieverts/h)

fac = normalization factor for dose (acr is also accepted instead of fac).
fac = -1 = normalize results to Q = 20 by dividing the parametric form of Q [5.0+17.0*exp(-(ln(2E))*2/6)] from ICRP60 (1990), paragraph A12.
fac = -2 = apply LANSCE albatross response function.
Default: fac = 1.0.

int = "log" or "lin" results in "log" or "lin" interpolation of energy; the dose function is always linear. That is, "lin" results in "linlin" interpolation, and "log" results in "loglin" interpolation.

Default: for ic = 10, 40: log
for ic = 20,31-39: recommended analytic parameterization.

ic = i = standard dose function.

<u>i neutron dose function</u>
10 = ICRP-21 1971
20 = NCRP-38 1971, ANSI/ANS-6.1.1-1977
31 = ANSI/ANS-6.1.1-1991 (AP anterior-posterior)
32 = (PA posterior-anterior)
33 = (LAT side exposure)
34 = (ROT normal to length and rotationally symmetric)
40 = ICRP-74 1996 ambient dose equivalent

<u>i photon dose function</u>
10 = ICRP-21 1971

20 = Claiborne & Trubey, ANSI/ANS 6.1.1-1977
31 = ANSI/ANS-6.1.1-1991 [AP (anterior-posterior)]
32 = PA (posterior-anterior)
33 = (LAT side exposure)
34 = (ROT normal to length and rotationally symmetric)
35 = (ISO isotropic)

Default: ic = 10

Examples:

DF4

DF0 ic 40 iu 1 lin fac 123.4

DF1 iu=2 acr=-2 log ic=34

4.2. Lattice Tally Speedup (F)

With no change in user interface, input files with large lattice tallies now run 10–1000 times faster if the following apply:

- The lattice is specified fully on the cell fill card, e.g., FILL –50:50 –50:50 –50:50.

- The tally chain refers to no more than one cell at each level, except for the lattice cell, which must include the entire range of all indices specified on the corresponding FILL card:

F4:p (1 < 2 < 3[–50:50 –50:50 –50:50] < 4).

The following will not work:
F4:p (1 < 2 < 3[–50:50 –50:50 –50:50] < 4 5)

because two cells, 4 and 5, were specified at the top level.

Example:

The following simple input file runs 70 times faster with MCNPX than with MCNPX 2.4.0 and MCNP4C versions:

```
21x21x21 void lattice of balls
11 0 -31 u=1 imp:p=1
12 0  31 u=1 imp:p=1
16 0 -32 u=2 imp:p=1
     lat=1 fill= -10:10 -10:10 -10:10 1 9260R
17 0 -33 fill=2 imp:p=1
18 0  33        imp:p=0
```

```
31 sph 0 0 0 .5
32 rpp -1 1 -1 1 -1 1
33 rpp -21 21   -21 21   -21 21

mode    p
print
prdmp 2j -3
sdef
nps    10000
f4:p (11<16[-10:10 -10:10 -10:10]<17)
```

Larger lattices and nested lattices offer even more dramatic speedups but take longer to demonstrate than the simple example shown.

4.3. Radiography Tally (FIP, FIR, FIC)

Radiography tallies may be input with either the standard MCNPX card names (PI, TIR, TIC) or the MCNP5 card names (**FIP, FIR, and FIC**). In all cases the radiographical plane is specified with C and FS cards for the s- and t- axes. The tally number is n and the particle type is p, which may be either neutron, N, or photon, P.

4.3.1. Pinhole Radiography

FIPn:p *X1 Y1 Z1 R0 X2 Y2 Z2 F1 F2 F3*

PIn:p *X1 Y1 Z1 R0 X2 Y2 Z2 F1 F2 F3*

X1 Y1 Z1 = coordinates of pinhole

R0 = 0

X2 Y2 Z2 = reference coordinates (center of object)

F1 = collimator radius

F2 = pinhole size

F3 = distance from pinhole to detector grid defined by C and FS cards.

4.3.2. Transmitted Image Projection

Rectangular grid:

FIRn:p *X1 Y1 Z1 R0 X2 Y2 Z2 F1 F2 F3*

TIRn:p *X1 Y1 Z1 R0 X2 Y2 Z2 F1 F2 F3*

Cylindrical grid:

FICn:p *X1 Y1 Z1 R0 X2 Y2 Z2 F1 F2 F3*

TICn:p *X1 Y1 Z1 R0 X2 Y2 Z2 F1 F2 F3*

X1 Y1 Z1 = coordinates of center of grid defined by C and FS cards

R0 = 0

X2 Y2 Z2 = reference coordinates (center of object)

F1 = -1 / 0 = scattered only / direct + scattered – contributions to detector

F2 = radial field of view

F3 = 0 / -1 contributions scored at center / random - on grid

4.4. Photonuclear and Proton Reaction Multipliers (FM)

Photonuclear and proton cross sections may be used in tally multipliers on the FM card. For example,

```
M102 92235 1 pnlib=27u
F2:P 1
FM2   (-1 102 18 1018)
```

Photonuclear cross-section reaction numbers are all positive, unlike the photoatomic reaction numbers, which are negative. The principal photonuclear cross sections are the following: 1 = total, 2 = nonelastic, 3 = elastic, 4 = heating, and >4 = various reactions such as 18 = (γ,f). The photonuclear yields (multiplicities) for various secondary particles are specified by adding 1000 times the secondary particle number to the reaction number. For example, 31001 is the total yield of deuterons (particle type d = 31); 34001 is the total yield of alphas (particle type α = 34); and 1018 is the total number of neutrons (particle type n = 1) from fission.

Proton reaction numbers are similar to the neutron reaction numbers: all positive. The principal proton cross sections are the following: ±1 = total, ±2 = nonelastic, ±3 = elastic, ±4 = heating, >4 = various reactions. On the LA150H proton library, the only available reaction is mt = 5 and its multiplicities, 1005, 9005, 31005, etc. The multiplicity reaction numbers are specified by adding 1000 times the secondary particle number to the reaction number. For interaction reaction mt = 5, the multiplicities are 1005 for neutrons, 9005 for protons, 31005 for deuterons, etc. The proton multiplicity, mt = 9001, 9004, 9005, etc., is generally available, along with the total cross-section and heating number, mt = 1, mt = 4.

It is always wise to plot the desired cross sections first to see if they are available with the expected reaction numbers in the data library. The tally multipliers treat the data the same as the data are treated in transport: the cross section at the lowest energy is extended down to E = 0 for protons with mt < 0; the cross section at the highest energy of the table is extended to E = ∞ for proton interaction cross sections with mt < 0, and for photonuclear interaction cross sections, mt < 1000. These extrapolations can be seen in the cross-section plots.

4.5. Expanded Cosine Specification (C)

Cosines now may be specified in degrees. They now also may be specified with surface flux (F2) tallies as

*C2 150 120 90 60 30 0 .

The * on the C2 card interprets cosines as in degrees. Entries must be such that the cosine is monotonically increasing.

4.6. Pulse-Height Light Tally with Anticoincidence: FT8 PHL

A new FT option is available for pulse-height (F8) tallies, which allows the F8 tally to be based on energy/light deposition in one or two other regions as specified via one or two F6 tallies. Thus, this tally is dependent on results from another tally, which works because the F8 tally is posted at the end of the particle history where the F6 tallies are accumulated along each track of the particle history. The format of the FT PHL card is

FT8 PHL N T_{A1} B_{A1} T_{A2} B_{A2} ... M T_{B1} B_{B1} T_{B2} B_{B2} ... ,
where

N = number of F6 tallies for the first detector region,

T_{A1} B_{A1} ... = pairings of tally number and f-bin number for the N F6 tallies of the first detector region,

M = number of F6 tallies for the second detector region, and

T_{B1} B_{B1} ... = pairings of tally number and f-bin number for the M F6 tally of the second detector region.

When M is nonzero, indicating the use of two detector regions, an FU card is required for the F8 tally. The entries on the FU card are presented in units of electron equivalent light (MeV_{ee}) and must increase monotonically. The particle type indicated on the F8 tally does not matter because this tally allows a combination of light output from various particle types. If B_{An} is zero, then the number of cell bins on the F8 card must match that on the corresponding T_{An} tally card. Setting B_{An} to zero allows for a lattice pulse-height PHL tally.

Examples

```
Case 1
        F8:n 5
        FT8  PHL 1 6 1 0
        E8   1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0
        F6:e 5
        DE6  LIN 1.0 1.5 2.0 2.5 3.0 3.5 10.0
        DF6  LIN 1.0 1.1 1.2 1.3 1.4 1.5 1.6
        FT6  GEB A B C

Case 2
        F8:n 5
        FT8  PHL 1 6 1 1 16 1
        E8   1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0
        FU8  1.5 2.5 3.5 4.5 5.5 6.5 7.5 8.5
        F6:e 5
        DE6  LIN 1.0 1.5 2.0 2.5 3.0 3.5 10.0
        DF6  LIN 1.0 1.1 1.2 1.3 1.4 1.5 1.6
        FT6  GEB A B C
        F16:e 6
        DE16 LIN 1.0 1.5 2.0 2.5 3.0 3.5 10.0
        DF16 LIN 1.0 1.1 1.2 1.3 1.4 1.5 1.6
        FT16 GEB A B C
```

In both cases, the F6 tallies convert energy deposition to equivalent light (units in millielectron volts). SD cards are not required with the F6 tallies as these divisors renormalize only the printed output for the F6 tallies and not the values stored in the tally arrays (thus, the F8 tally will result in the same value, regardless of whether the F6 tally has an SD card). The DE/DF conversion is based on the incident particle energy, and the values on the DF card should be the dL/dE for that incident particle energy. Thus, the F6 tally will multiply the dL/dE values by the energy deposition to give the light output (ΔL) summed over each track. Also, no energy bins exist for the F6 tallies. The F8 tally uses the total light output. Energy bins (E6 card) can be added, but the F8 tally will use the value from the total bin. Similarly, for other bins associated with the F6 tally, in each case the TFC bin is used to extract the value for the F8 tally (see the TF card to alter this). The FT GEB cards are used to perform Gaussian broadening on these tally values; however, this is done only at the end of the particle history to determine the light output value used in the pulse-height tally.

In Case 1, the electron light output from only one region (cell 5) is used to subdivide the pulse-height tally. In this case, a pulse of 1 (input source weight) is put into the first E8 bin when the light output in cell 5 is <1 MeV. It is placed in the second E8 bin when the light output is between 1 and 2 MeV, etc. A zero F6 tally will result in no F8 tally.

In Case 2, the light output from two regions (cells 5 and 6) is used to subdivide the pulse-height tally. This case is useful for coincidence/anticoincidence applications. A pulse of 1 (input source weight) is put into the first E8 bin and into the first FU8 bin when the light output in cell 5 is <1.0 MeV *and* the light output in cell 6 is <1.5 MeV. This pulse is put into the first E8 bin and into the second FU8 bin when the light output in cell 5 is <1.0 MeV *and* the light output in cell 6 is between 1.5 and 2.5 MeV. A zero light output in both cells will result in no F8 tally. A zero light output in cell 5 (tally 6) with a nonzero light output in cell 6 (tally 16) will result in a pulse

in the corresponding FU8 bin. Similarly, for a zero light output in cell 6 and a nonzero light output in cell 5, a pulse will be put into the corresponding E8 bin. Note that the E8 and FU8 bins do not have to be the same and typically would not be unless the detector regions were of similar material and size. Separate F6 tallies (as in Case 2, F6 and F16) are needed only when the two regions have different light conversion functions. If the two regions are of the same material, then a single F6 tally can be used as follows.

```
F8:n 5
FT8  PHL 2 6 1 6 2 0
E8   1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0
FU8  1.5 2.5 3.5 4.5 5.5 6.5 7.5 8.5
F6:e 5 6
DE6  LIN 1.0 1.5 2.0 2.5 3.0 3.5 10.0
DF6  LIN 1.0 1.1 1.2 1.3 1.4 1.5 1.6
```

Currently, it is not important what cell is listed on the F8 card because this tally is made only at the end of a particle history and depends only on the tally results of the listed F6 tallies. Having multiple cells listed on the F8 card is meaningful only when the f-bin parameter (i.e., B_{An} or B_{Bn}) of the FT PHL option is zero, indicating a lattice grid of detector regions. Otherwise, each additional F8 cell bin simply will be a duplicate of the first cell bin.

4.7. Coincidence Capture Tally (FT8 CAP)

The FT8 capture tally scores the number of captures in specified combinations of nuclides at the end of each history. It is particularly for neutron coincidence detectors. In addition, captures may be written to an auxiliary output file, PTRAC. Section XXX describes the PTRAC capture file.

FT8 [-Mc] [-Mo] I1 I2 …

Where Mc = optional maximum number of captures (default = 21)
Mo = optional maximum number of moments (default = 12)
In = capture nuclides such as 3006 or 5010 for ^{6}Li or ^{10}B.

Example:

```
F8:n    2 (5 6) 7 T
FT8     cap     3006    5010
T8   1  7LOG  1E8   .
```

In this example, captures and moments are tallied in cells 2, 7, in the combination of 5 and 6, and in the total over cells 2, 5, 6, 7. The captures by either ^{6}Li or ^{10}B are tallied. Results are tabulated in time bins at 1, 10, 100, 1000, 1e4, 1e5, 1e6, 1e7, and 1e8 shakes—that is, in the range of 10 nanoseconds to 1 second.

4.7.1. Restrictions

Coincidence counting of capture multiplicities and moments requires analog capture: CUT:N 2J 0 0. Calculations must be totally analog with no variance reduction. Fission multiplicity is also

required: PHYS:N J 100 3J –1. Variance reduction is not allowed. An FT8 CAP tally in an input file will automatically set analog capture, fission multiplicity, and exit with error messages if there is variance reduction. The capture multiplicities and moments are stored in 80 cosine bins, which are printed out with the F8 tally. A much more readable table of capture multiplicities and moments is given in Print Table 118. The captures and moments can be compared to Print Table 117, which has the spontaneous fission source and induced fission summaries of fission neutrons and moments.

The capture tallies may be written to a PTRAC file for further analysis by auxiliary codes. See the section on the PTRAC card extensions.

The presence of "cap" on the FT8 card forces CUT:N 2J 0 0, which specifies neutron analog capture. The capture multiplicities and moments are stored in 80 cosine bins, which are printed out with the F8 tally. A much more readable table of capture multiplicities and moments is given in Print Table 118.

4.7.2. Interpreting Capture Tally Output

The FT8 CAP coincidence capture tally option produces both a standard tally, which is generally unreadable, and a coincidence capture table, print table 118. An example is now provided to help in the interpretation of this table.

```
neutron captures, moments & multiplicity distributions. tally 8 print table
118

 cell:    999

 neutron captures on 3he
                      captures      captures    multiplicity fractions
         histories   by number     by weight    by number    by weight   error

 captures =  0     700        0   0.00000E+00  7.00000E-02  3.25400E-02  0.0364
 captures =  1    2285     2285   1.06220E-01  2.28500E-01  1.06220E-01  0.0184
 captures =  2    3223     6446   2.99647E-01  3.22300E-01  1.49823E-01  0.0145
 captures =  3    2489     7467   3.47109E-01  2.48900E-01  1.15703E-01  0.0174
 captures =  4    1022     4088   1.90033E-01  1.02200E-01  4.75084E-02  0.0296
 captures =  5     209     1045   4.85775E-02  2.09000E-02  9.71551E-03  0.0684
 captures =  6      51      306   1.42246E-02  5.10000E-03  2.37077E-03  0.1397
 captures =  7      12       84   3.90480E-03  1.20000E-03  5.57828E-04  0.2885
 captures >  7       9       73   3.39345E-03  9.00000E-04  4.18371E-04  0.3332

    total        10000    21794   1.01311E+00  1.00000E+00  4.64857E-01  0.0056

      factorial moments              by number               by weight

             3he                 2.17940E+00 0.0056      1.01311E+00 0.0056
        3he(3he-1)/2!            2.01890E+00 0.0128      9.38499E-01 0.0128
     3he(3he-1)(3he-2)/3!        1.06390E+00 0.0291      4.94561E-01 0.0291
  3he(3he-1) .... (3he-3)/4!     3.93800E-01 0.0744      1.83061E-01 0.0744
  3he(3he-1) .... (3he-4)/5!     1.34100E-01 0.1636      6.23373E-02 0.1636
  3he(3he-1) .... (3he-5)/6!     4.43000E-02 0.2666      2.05932E-02 0.2666
```

```
  3he(3he-1) .... (3he-6)/7!    1.12000E-02 0.3808      5.20640E-03 0.3808
  3he(3he-1) .... (3he-7)/8!    1.70000E-03 0.5548      7.90257E-04 0.5548
```

The capture tally input for this problem was:

```
      F8:n   999                          input F8 card
      FT8    CAP   -8      -8      2003   input FT8 CAP card
```

Note that the line captures > 7 9 73 indicates 9 histories had 8 or more neutrons captured. This implies that 8 histories had 8 x 8 = 64 neutrons captured and 1 history had 1 x 9 neutrons captured for a total of 73 neutrons captured. The table of captures was evidently too short and the problem should have been run with FT8 CAP -9 -9 or even more captures and moments. This only affects the captures > 7 line and the error estimate on the totals capture line; all other information is correct as if more captures and moments were listed.

Now for an interpretation of the neutron captures on 3he table.

Column 1 is the number of histories according to the number of captures by the designated material (2003 = 3he) in the designated cell (999) This sums to the total number of source histories for the problem, nps = 10000.

Column 2 is the number of captures by 2003 in cell 999 = 21794 Because analog capture is the default for F8 tallies, the total weight captured is also 21794.0.

Column 3 is the total weight captured divided by the tally normalization. For SDEF PAR = -SF the tally normalization is the number of source histories = number of spontaneous fissions = 10000. For SDEF PAR = -SF column 3 would be 21794.0 / 10000 = 2.17940. In this problem, SDEF PAR = SF, and the tally normalization is the source particles = spontaneous fission neutrons = 21512. Thus captures by weight is 21794.0 / 21512 = 1.01311.

Column 4 is the multiplicity fraction by number which is column 1 divided by the number of source histories. The total is always 1.00000.

Column 5 is the multiplicity fraction by weight, which is the weight of histories undergoing capture, divided by the tally normalization. For SDEF PAR = -SF this would be 10000.0 / 10000 = 1.00000. In this problem, SDEF PAR = SF and the multiplicity fraction by weight is 10000.0 / 21512 = .464857.

The interpretation of the factorial moments table now follows.

The first moment by number is the number of captures divided by the number of source histories = 21794 / 10000 = 2.17940.

The first moment by weight is the total weight of capture divided by the tally normalization. For SDEF PAR = -SF this would be 21794.0 / 10000 = 21794.0. In this problem SDEF PAR = SF and the first moment by weight is 21794.0 / 21512 = 1.01311.

The second moment is N*(N-1)/2 where N is the number of captures. In this problem,

N	N*(N-1)/2		histories		product
1	0	x	2285	=	0
2	1	x	3223	=	3223
3	3	x	2489	=	7467
4	6	x	1022	=	6132
5	10	x	209	=	2090
6	15	x	51	=	765
7	21	x	12	=	252
8	28	x	8	=	224
9	36	x	1	=	36
sum				=	20189

The second moment by number is divided by the number of histories:

20189 / 10000 = 2.01890

Because of analog capture, the second moment weight is 20189.0 The second moment by weight is divided by the tally normalization. For SDEF PAR = -SF this would be 20189.0 / 10000 = 2.01890, which is the same as the second moment by number. In this problem, SDEF PAR = SF and the second moment by weight is:

20189.0 / 21512 = .938499

The 7th moment is:

7x6x5x4x3x2x1/7!	=	1	x	12	=	12
8x7x6x5x4x3x2/7!	=	8	x	8	=	64
9x8x7x6x5x4x3/7!	=	36	x	1	=	36
sum					=	112

Thus 112 / 10000 = .0112

The 8th moment is:

8x7x6x5x4x3x2x1/8!	=	1	x	8	=	8
9x8x7x6x5x4x3x2/8!	=	9	x	1	=	9
sum					=	17

Thus 17 / 10000 = .0017

And the 9th moment is:

9x8x7x6x5x4x3x2x1/9!	=	1	x	1	=	1

Thus 1 / 10000 = .0001

4.7.3. Possible Future Extensions of FT8 CAP Option

The coincidence counter capture tally model lacks many standard tally features to make the algorithm faster. Adding the following tally capabilities would be a straightforward extension:

- extension to particle types other than neutrons,
- tally cell and surface flagging,
- extension to other special tally treatment options on the FT card,
- tally segmenting,

- tally multipliers, and
- energy bins.

4.8. Residual Nuclei Tally: FT8 RES

Residual nuclei from nuclear interactions in the model physics energy range may be tallied with the FT tally special treatments RES option in conjunction with pulse-height tallies. The form of the FT card is

FT8 **RES**

or

FT8 **RES** Z_1 Z_2 .

The interaction of high-energy particles with target nuclei causes the production of many residual nuclei. The generated residual nuclei can be recorded to an F8 tally if used with an FT8 RES special treatment option. The residuals are recorded at each interaction in the model physics; residual nuclei are not tabulated at collisions utilizing table physics.

By default, the FT8 RES card will cause the corresponding F8 tally to have 2000+ user bins for each possible residual nucleus ZAID. The range of ZAID bins may be reduced by specifying Z_1 and Z_2, which correspond to a range of possible Z values. If Z_1 and Z_2 are specified and a residual is generated with a higher or lower Z, the residual will not be scored in the F8 tally.

The FT8 RES capability is particularly useful with the eighth LCA card entry, NOACT.
When NOACT = –2 on the LCA card, then the source particle immediately collides in the source material. All subsequent daughter particles then are transported without further collision, as if in a vacuum. The F8 tally with an FT8 RES special tally treatment is then simply the distribution of nuclides resulting from a single collision.

The following input files model a 1.2-GeV proton source having a single collision with ^{208}Pb.

```
Test of p(1.2GeV)+Pb(208)
1 1 -11. -1 imp:h 1
2 0        1 imp:h 0

1 so .01

mode h n
sdef par h erg=1200 vec 0 0 1 dir 1
m1 82208 1
phys:h 1300 j 0
phys:n 1300 3j 0
nps 10000
f8:h 1
ft8 res 1 99
fq8 u e
lca   2 1 1 23 1 1 0 -2 0
```

These data may be plotted with MCNPX using the tally plotter and the following execute line command:

MCNPX Z

where the command file, COM91, is

```
rmctal=mctl91
tally 8 free u xlim 81189 8120 ylim .0001 .01
```

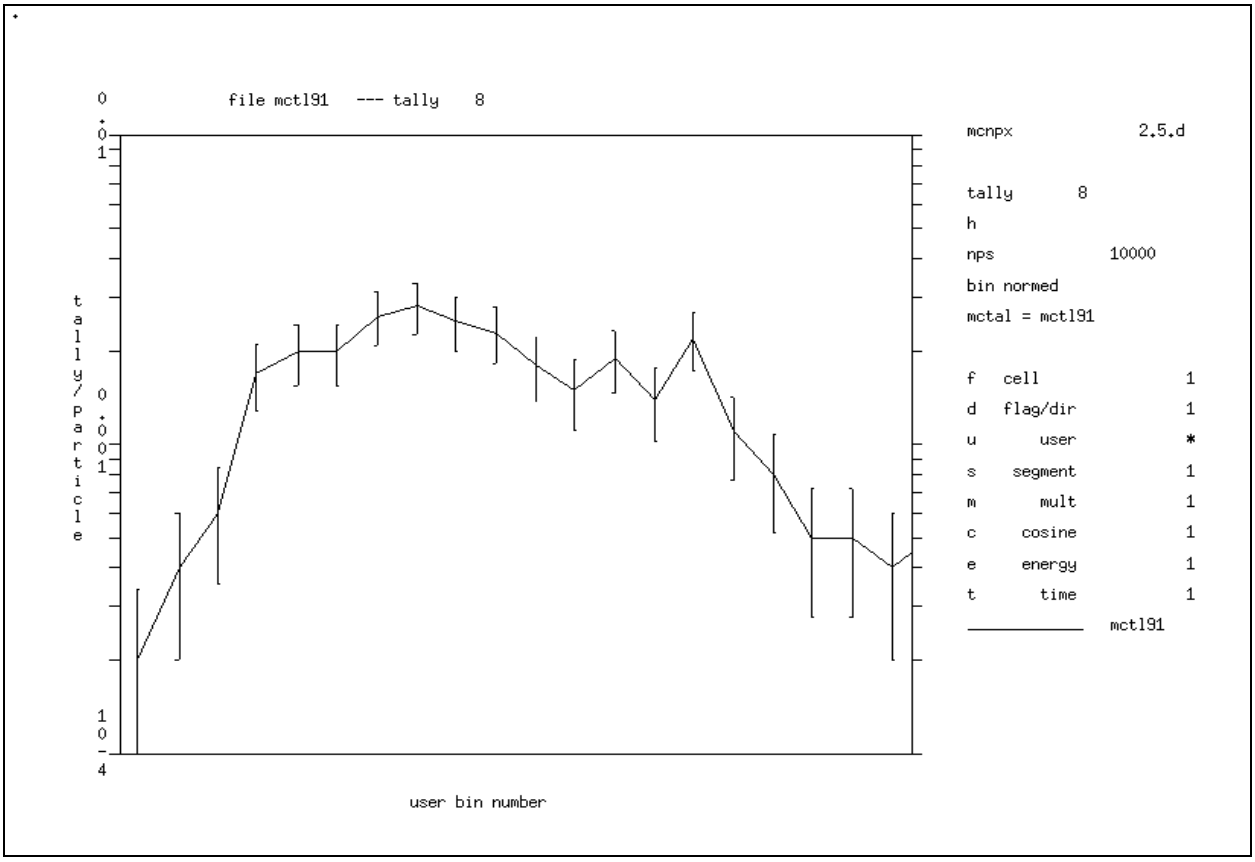


Fig. 4. Residuals for $_{81}$T1 isotopes 189–201 from 1.3-GeV protons on $^{208}_{82}$Pb.

5.0. OTHER INPUT FILE EXTENSIONS

- Logarithmic interpolation on input cards;
- Auxiliary input files (READ);
- HISTP file size control (HISTP);
- DXTRAN/detector underflow control (DBCN);
- PTRAC file for coincidence counting (PTRAC).
-

5.1. Logarithmic Interpolation

Logarithmic interpolation is now allowed on all input cards where lists of numbers are given. It is similar to the IJMR interpolation. For example,

E0 1.e-3 6log 1.e4

is interpreted as

E0 .001 .01 .1 1 10 100 1000 10000 .

5.2. Auxiliary Input File and Encryption

The new MCNPX READ card enables

- the reading of parts of the input file from other (auxiliary) files,
- the suppression of the printing of the auxiliary input files to shorten output files and protect proprietary information, and
- the encryption of auxiliary input files to protect proprietary information.

The READ card may appear anywhere after the title card of an MCNPX input file, but not in the middle of a card continuation.

5.2.1. Reading from an Auxiliary File

READ FILE = *filename*

will cause input from the file "*filename*" to be inserted after the READ command in the MCNPX input deck. Unlike most MCNPX input cards, there may be as many READ cards and auxiliary input files as desired.

5.2.2. Suppressing Input Printing

READ NOECHO

will suppress printing of the input cards following the READ card. The echoing of input cards is resumed with

READ ECHO .

Whereas the default of the READ card is ECHO, the echoing will resume when the next READ card is encountered without the NOECHO command.

The echoing of the input cards also is resumed when an "end of file" is encountered.

READ FILE = *filename* NOECHO

causes the input from the auxiliary file, *filename,* to be suppressed. After the file *filename* is read, input transfers back to the input file with the READ card and printing is no longer suppressed.

5.2.3. Encryption of Input

A simple encryption scheme is available in MCNPX. The encryption capability can be used to protect proprietary designs of tools and other systems modeled with MCNPX. To read an encrypted file,

READ DECODE *password* FILE = *filename* .

The encrypted input file will not be echoed, and many default print tables are turned off (and cannot be turned back on) to protect the data in the encrypted file.

To write an encrypted file,

READ ENCODE *password* FILE = *filename* .

The encryption capability is localized in subroutine ENCRYPT. The MCNPX scheme is very simple; therefore, it protects nothing. To protect input, the subroutine should be modified to a more sophisticated scheme known only to those producing the data, and only executable MCNPX versions should be provided to users of the encrypted files.

5.3. HISTP File size control

HISTP is the card that controls the writing of information to an external file for analysis by the HTAPE3X program. HISTP can take two different argument types:

HISTP –lhist icl_1 icl_2 icl_3 .

lhist is the parameter that controls the number of words written to a *histp* file. Once this limit is exceeded, a new file will be written with the name *histpa*, and the incrementing of the name continues until all particles are run. lhist must be entered as a negative number and may appear anywhere on the card. The default value of lhist is 500,000,000 words.

icl_1, icl_2, … are cell numbers. If no icl value is present, all events will be written to *histp*. The user may enter as many icl values as needed, and only events within these cells will be written to *histp*.

Example:

HISTP –100000 5 6 3 10 .

Each *histp* file will contain a maximum of 100,000 words. Only events within cells 3, 5, 6, and 10 will be written to the *histp* file.

HISTP

Each *histp* file will contain a maximum of 500,000,000 words (which virtually ensures that only one file will be written). All events in all cells will be written to the file.

Note: writing *histp* files during multiprocessing is still under development.

5.4. Detector/DXTRAN Underflow control (DBCN)

DXTRAN and point detector contributions are based on the next-event estimator that makes contributions of

$$W * p(\mu)*\exp(\lambda) / 2\pi R^2$$

Where W = particle weight

$p(\mu)$ is the density function for scattering to the detector or DXTRAN sphere

R is the distance from collision to the detector or DXTRAN sphere

λ is the attenuation factor, namely the sum of total macroscopic cross section times track length for each material region crossed between the collision and detector or DXTRAN sphere.

In MCNP4C, if $\lambda > 80$, then $\exp(\lambda) = 0$, and the score is terminated as "underflow in transmission." These small contributions are truncated That is, they are neglected, which biases answers by omitting them Generally, they are insignificant to the final answer. But in some cases, the underflow contribution is significant and needed. And when DXTRAN spheres or point detectors are used to get tally contributions for generating weight windows, sometimes these underflow contributions cannot be neglected.

It is now possible to specify the underflow limit with the 6^{th} entry on the DBCN card. The default is 80, but values between 50 – 200 are now accepted.

If DXTRAN/detector underflow is significant in your calculation, generally you have serious problems like not sampling enough collisions near the detector. Changing the underflow limit should be done only with extreme caution.

5.5. PTRAC Capture File (PTRAC)

The FT8 CAP coincident capture tallies may be written to a PTRAC file for further analysis by auxiliary codes. A PTRAC file is created with the following MCNPX input file (INP) input card:

PTRAC *EVENT = cap* *FILE = asc*

Either an ascii (text) file (*FILE = asc*) or a binary file (*FILE = bin*) may be created. The default is a binary file.

For *EVENT = cap,* most of the standard PTRAC capabilities are bypassed (for speed), and the data written to each line (or binary file record) is very different from the usual PTRAC data.

5.5.1. History Information on PTRAC file

For binary files, the entries on each line are

NPS Time Cell

For ascii files, the entries on each line are (format: i10,1p1e15.5,2i8)

NPS Time Cell Source ,

where

NPS = particle history number,
time = time from source event to analog capture in any FT8 cap tally,
cell = cell in which analog capture occurred, and
source = source particle number of a given history.

For example, after the usual PTRAC header, the capture events would be recorded as

NPS	Time	Cell	Source
1	4.5e01	22	4
1	0.0e00	0	3
1	2.6e02	−22	2
1	3.5e02	−22	2
1	1.5e00	23	2
1	0.0e00	0	1
3	0.0e00	0	2
3	0.0e00	0	1

In the previous example, source history 1 (NPS = 1) had four spontaneous fission neutrons (4, 3, 2, 1 in the Source column). The fourth (Source 4—numbering is done as in the MCNPX bank: last in, first out) was captured in Cell 22 at Time = 45 shakes after the source spontaneous fission. The third (Source 3) was not captured (Time = 0.0, Cell = 0). The second (Source 2) caused an induced fission—or possibly several induced fissions—as flagged by the negative cell number. Captures in Cell 22 were at 260 and 350 shakes for these neutrons from induced fission (from the second neutron from a spontaneous fission). The second spontaneous fission neutron was captured in cell 23; this neutron must have been a branch [after an (n,2n) split perhaps] that did not undergo fission. The final (first, Source 1) spontaneous fission neutron was not captured.

The second history (NPS = 2) is a spontaneous fission of multiplicity zero; thus, there is no history 2.

The third source particle history is a fission that results in two fission neutrons (Source = 2, Source = 1), neither of which is captured.

For binary files (*FILE = bin*), only three words per record are written. In the fourth column, "Source" is omitted.

5.5.2. Changing the Name of the PTRAC File

The PTRAC file name may be changed on the MCNPX execution line:

mcnpx *ptrac = filename*

and the file name will be altered if an old file by that name already exists. For example, if file *ptraca* was the last PTRAC file, then the created PTRAC file would be *ptracb.*

5.5.3. Possible Future Extensions of the PTRAC Capture Option

Many standard PTRAC capabilities are missing from the PTRAC capture tally output file capability. These could be added, if desired, and could include nearly all of the remaining PTRAC options: BUFFER, MAX, MEPH, WRITE, other EVENTs, FILTER, particle type, NPS, cell, surface, tally and VALUE.

6.0. GRAPHICS

MCNPX has geometry, tally, and cross section plotting extensions:

- Enhanced color geometry plots;
- i,j,k lattice indexing in geometry plots;
- Geometry plot of weight window generator superimposed mesh;
- 2D color tally contour plots, including lattices and radiography;
- Proton and photonuclear cross-section plots;
- Pause command for tally and cross-section plots.

6.1. Sixty-Four-Color Plotting and Shading by Cell Parameters

MCNP4C3 had 10 plotting colors; MCNPX now has 64-color plotting. Shading of geometry plots may be used for any cell parameter. MCNP4C colored its geometry plots by material only, giving a different color to each material number. MCNPX can now color geometry plots by any cell quantity. Each cell can have a different color, or each repeated structure level or universe can have a different color. Logarithmic shading of importances, weight windows, and summary information is automatic. If a superimposed weight-window mesh is used, coloring also may be done by the value of the mesh weight windows.

In the interactive capability, the "SCALES n" button has been moved up two lines (after the cursor) to make room for a larger "COLOR name" button. The default is "COLOR mat", which colors problem cells by the program material number. This button must be clicked to get "COLOR off" (black and white) and then clicked again to color by whatever parameter is listed after the "Edit" button. For example, in the right margin, click "cel", which will make the "Edit" quantity "cel". Next, click "COLOR" so that it says "COLOR cel"; on the next plot, the color shades will be determined by program cell number.

For command/prompt plotting, enter

PLOT> label 0 1 rho ;

the color command then must be set such as

PLOT> color on ,

and the coloring will now be by rho, the atom density.

6.2. I,J,K Lattice Index Labeling

The i,j,k lattice indices of repeated structures/lattice geometries now may be used as plot labels in geometry plots, as illustrated in Fig. 1.

If the level (LEVEL command or button) is not a lattice cell level, then the indices will be for the next lattice in a higher level. To get the lattice index labels, choose ijk as the edit quantity by clicking ijk in the right margin. Then click the send entry after LABEL so that it reads “LABEL off ijk”. For command/prompt plotting, enter “Label 0 1 ijk”.

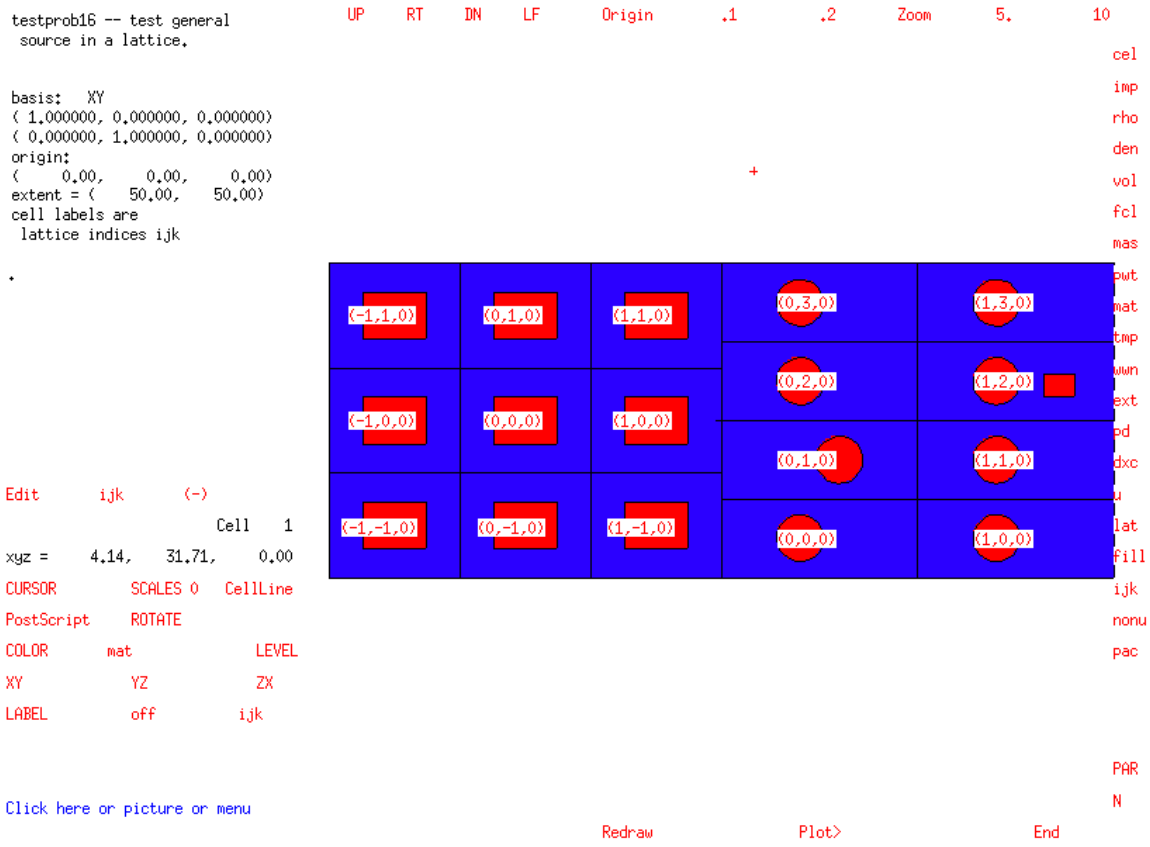


Fig. 1. Lattice indexing in geometry plot.

6.3. Weight Window Generator Superimposed Mesh Plots

MCNPX can plot the weight window generator (WWG) superimposed mesh specified on the MESH card in an input file MCNP4C3 and previous MCNPX versions could only plot the weight-window superimposed mesh used in a problem, and a WWINP file had to be provided In the MCNPX geometry plotter, toggle CellLine for the following options:

CellLine	Plot geometric cells, outlined in black
WW MESH	Plot the weight window superimposed mesh (WWINP required)
WW+Cell	Plot superimposed mesh and cells outlined in black
WWG MESH	Plot MESH card weight window generator mesh
WWG+Cell	Plot WWG mesh and cells outlined in black
No Lines	Plot cells not outlined in black

The CellLine and No Lines options are always available WW Mesh and WW+Cell are only available when the WWP card calls for using a superimposed weight window mesh (5^{th} entry negative) and a WWINP file is provided. WWG MESH and WWG+Cell are only available when a MESH card is in the input file and when the weight window generator requests superimposed mesh generation (WWG card 2^{nd} entry = 0) In all cases the cells may be outlined in black (CellLine, WW+Cell, WWG+Cell) or the cells may be simply colored without outlining (WW MESH, WWG MESH, No Lines.)

6.3.1. Geometry Plot of Weight-Window-Generator Superimposed Mesh

MCNPX can plot the weight-window-generator (WWG) superimposed mesh specified on the MESH card in an input file. The following options are now available.

0.	No Lines	Plot cells not outlined in black
1.	CellLine	Plot geometric cells, outlined in black
2.	WW MESH	Plot WW mesh (WWINP, WWP 4j –1 required)
3.	WW + Cell	Plot WW mesh (WWINP, WWP 4j –1 required) + CellLine
4.	WWG MESH	Plot WWG mesh (MESH, WWG J 0 required)
5.	WWG + Cell	Plot WWG mesh (MESH, WWG J 0 required) + CellLine

In the interactive MCNPX geometry plotter, toggle CellLine for the above options.

In the command-mode geometry plotter, the option is *mesh = n,* where *n* is the number 0–5, as determined by the options list above.

The ability to plot the WWG mesh, options *mesh = 4* and *mesh = 5*, is new in MCNPX 2.5.d.

The CellLine and No Lines options are always available. WW MESH and WW + Cell are available only when the WWP card calls for using a superimposed weight-window mesh (fifth entry negative) and when a WWINP file is provided. WWG MESH and WWG + Cell are available only when a MESH card is present in the input file and when the weight-window generator requests superimposed mesh generation (WWG card second entry = 0). In all cases, the cells may be outlined in black (CellLine, WW + Cell, WWG + Cell) or the cells simply may be colored without outlining (WW MESH, WWG MESH, No Lines).

6.3.2. Example

Input file: *inp10*

```
Demonstration of WWG Plot
1 1 1.0   -1  imp:p 1
2 0        1  imp:p 0

1 rcc 0 0 0  0 10 0  5

mode p
sdef sur 1.3 vec 0 1 0 dir 1 erg 100
m1 1001 2 8016 1
nps 1000
f1:p 1.2
wwg 1 0
mesh geom=cyl origin=0 -1 0  ref=0 .1 0  axs=0 1 0  vec=1 0 0
     imesh 6   iints 7  jmesh 12  jints 7   kmesh 1   kints 3
```

Com file: *com10*

```
ex 10 lab 0 0 px 0 mesh 4
pause
py 5
pause
```

mcnpx i = *inp10* com = *com10* ip

Or, instead of using the command file (with plot commands in command mode), the interactive plotter can be used.

mcnpx i = *inp10* ip

click	CellLine	to get WWG + Cell
	label sur	to turn off surface labels
	XY	to get px = 0 view (axial view, Fig. 1)
	Zoom 10	to get 10x magnification (click twice)
	Origin	click in the center of material to center picture
	ZX	to get py = 5 view (radial view, Fig. 2)

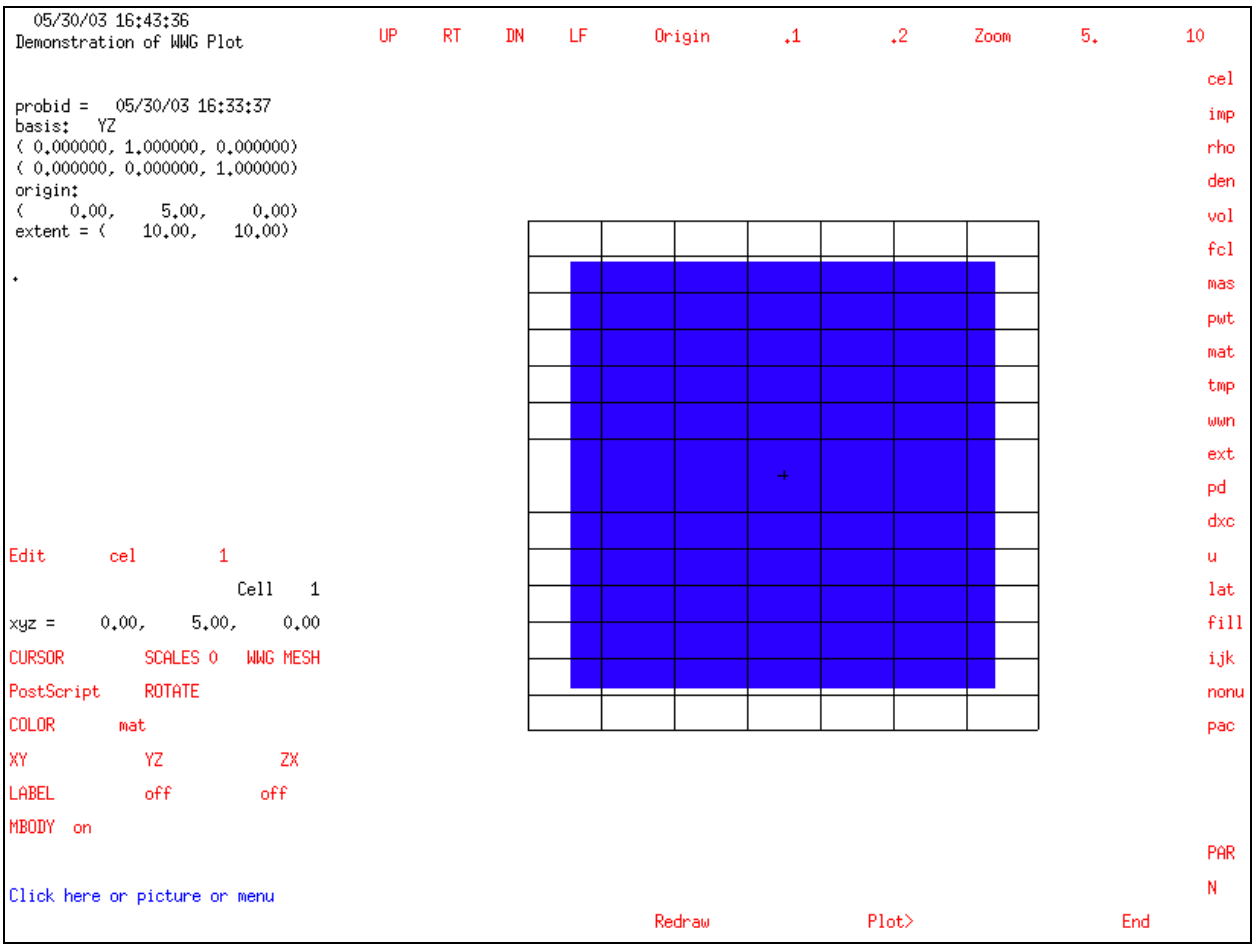


Fig. 1. WWG mesh plot, axial view.

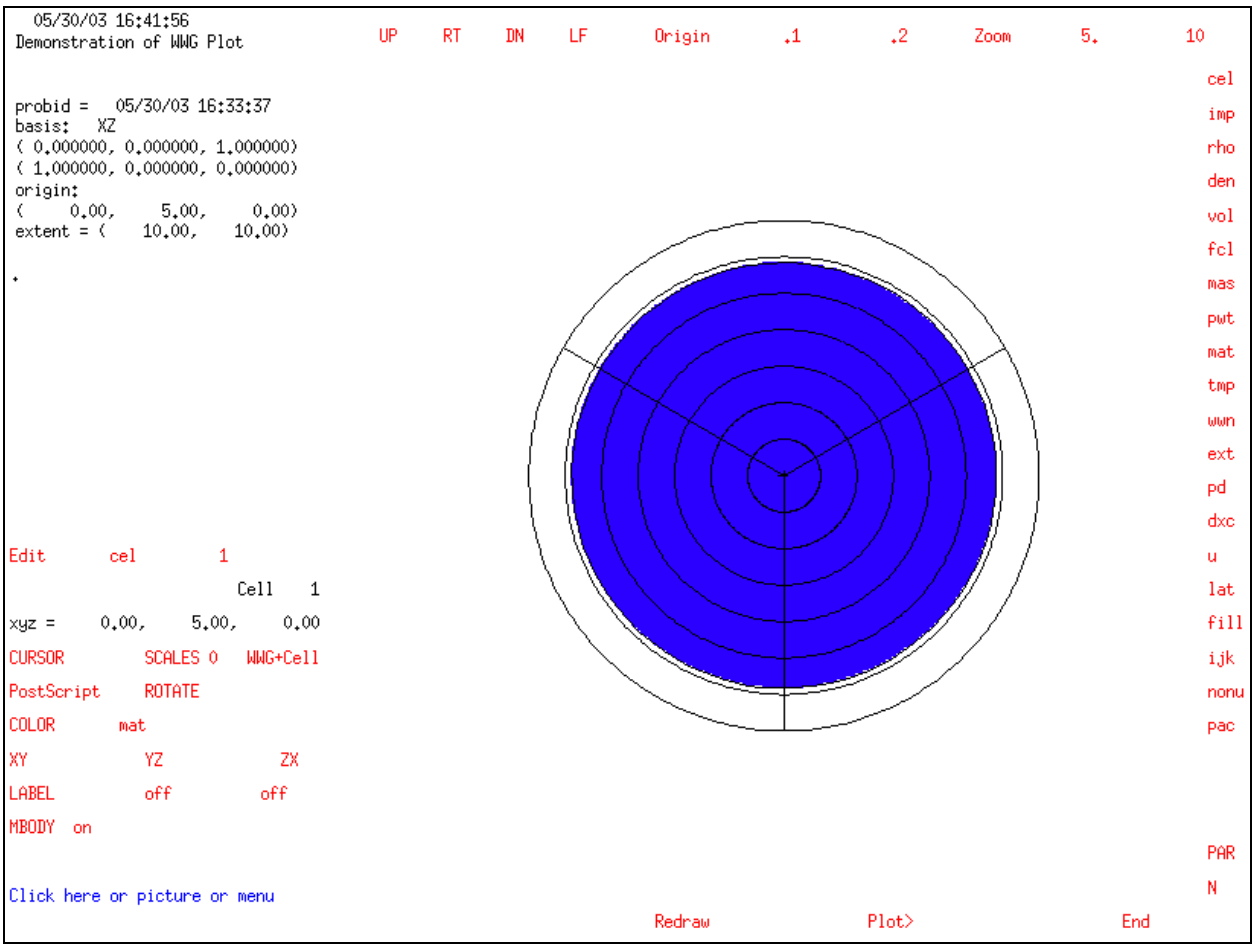


Fig. 2. WWG plot, radial view.

6.4. Color Contour Tally Plots

Tally output may now be plotted as 2D color contours from either MCTAL or RUNTPE files For example, a radiography tally with s- and t-axes specified on FS and C cards can be plotted with the MCNPX Z option as illustrated below. For the first time the I and J indices of I,J,K lattice tally plots can also have contour plots. We will extend the capability to mesh tally plots in a future MCNPX version.

6.4.1. Example

The following example is a radiograph of a 4-cm radius, 1-cm thick U238 disc with an embedded 2 mm void sphere The input file is:

```
Radiography Tally
1 5 -25.0  -1 3          imp:p=1
2 0         (1:-3) -2    imp:p=1
3 0         2            imp:p=0

1 RCC 0 0 0  0 0 1  4
```

```
2 RPP -1000 1000 -1000 1000 -1000 1000
3 SPH 2 0 1  .2

mode p
nps 100000 5
sdef pos=0 0 -20 axs=0 0 1 rad=d1 ext=0 vec=0 0 1 dir=d2 erg=6
si1 0 .1
sp1 -21 1
si2 -1 1
sp2 -31 1
m5 92238 1
print
prdmp 2j 1
tir5:p 0 0 10 0 0 0 -100 0 100 0
fs5    -10. 99i 10.
c5     -10. 99i 10.
```

To get the contour plot, run

MCNPX Z RUNTPE=*filename*

The contour plots may also be read from a MCTAL file instead of the RUNTPE. When the code gives you the MCPLOT prompt, enter two dimensions with the free command, for example, S and C:

MCPLOT> free SC

Recall that the tally dimensions are:

F	surface / cell / detector F card bin
D	total / direct or flagged bin
U	user bin
S	segment or radiography s-axis bin
M	multiplier bin
C	cosine or radiography t-axis bin
E	energy bin
T	time bin

The results are:

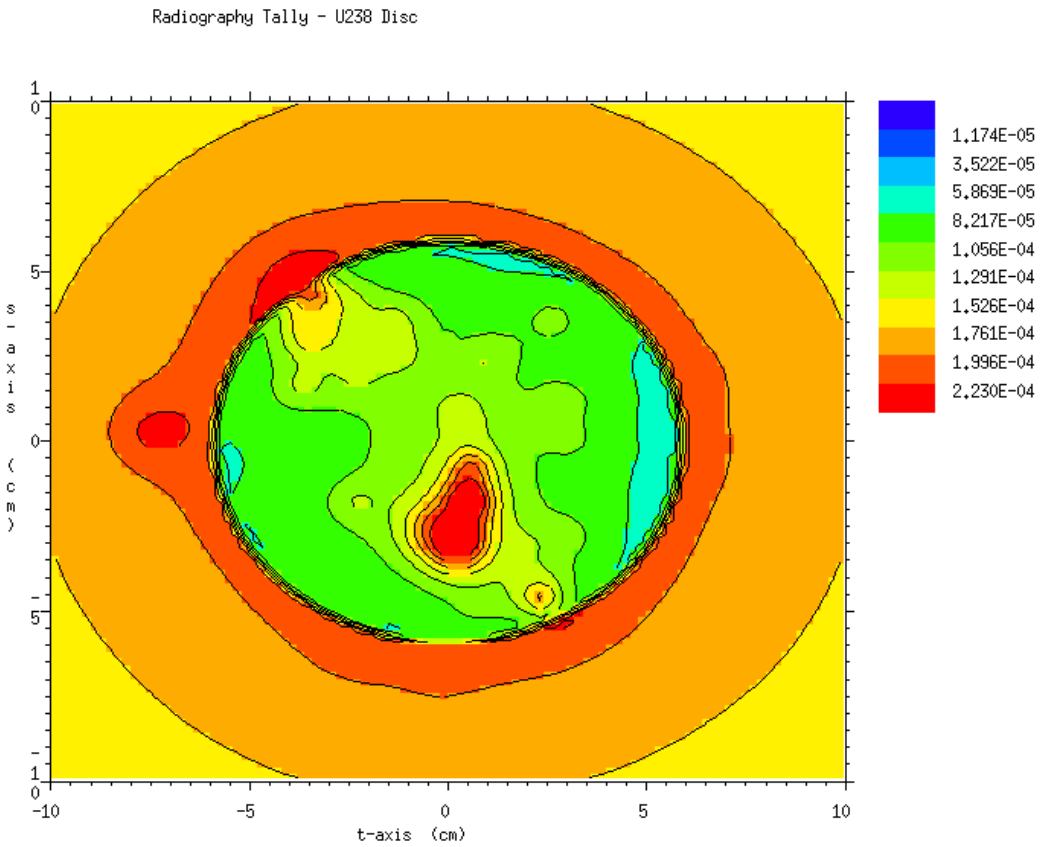


Figure 1: Scattered photon radiographic image of U238 disc

Although the picture is pretty, the embedded void sphere is not seen and the shapes in the symmetrical disc indicate poor convergence In a direct tally (MCPLOT command: fixed D 2) the embedded sphere is seen, but the picture is rather plain.

6.4.2. User Interface

6.4.2.1. MCPLOT FREE command

The MCPLOT free command works the same as always, but with the following extension:

FREE X[Y] **[nxm] [all]**

Variables x and y are tally bin indices (fdusmcet) or lattice indices (ijk) for lattice tally plots. Currently the lattice indices are limited to "i" or "ij" and the other indicies are specified using the "fix" command (see below). Specifying a single variable after the free command produces a 1-D plot Specifying two variables produces a 2-D contour plot. The remaining two keywords are valid only when x=i or xy=ij. The "nxm" keyword specifies the number of bins associated with the "i" and "j" lattice indices. The "all" keyword specifies that the minimum and maximum contour range should be take from all of the tally bins. Omitting this keyword results

in the default minimum and maximum contour range which includes only those tally values contained in the specified 2-D plot.

Example 1:

free i 64x64 fix j=38 fix k=30

This command specifies a 1-D lattice tally plot of the cell bins which should correspond to a lattice tally with 64 "i" index bins, 64 "j" index bins, and at least 30 "k" index bins. With the "k" index set to 30 and the "j" index to 38, the offset into the f-bins will be 29*64*64+37*64 = 121152. The minimum and maximum values will be determined from the 64 "i" bin values included in the plot. If the "j" and "k" indices are not specified, their default value of 1 is assumed which results in an offset of 0.

Example 2:

free ij 10x30 all fix k=60

This specifies a 10 by 30 2-D contour plot which should correspond to a lattice tally with 10 "i" bins, 30 "j" bins, and at least 60 "k" bins. Note the "k" index is specified using the "fix" command, which sets the offset into the f bins as 60*10*30 = 18000. In this case, the contour range is taken from all of the f-bin tally values.

6.4.2.2. MCPLOT FIXED command

The MCPLOT FIX command works the same as always, but has the following extension:

fix x=n

The keyword "x" is one of the tally bin indices (fdusmcet) as before. Or, it may now be one of the lattice indices (ijk) for lattice tally plots. The value of "n" specifies a bin value for that index. Currently, only the "j" and "k" indices are allowed for a 1-D ijk plot, and only the "k" index is allowed for a 2-D ijk contour plot.

6.4.2.3. MCPLOT CONTOUR command

The MCPLOT CONTOUR command has an additional optional keyword. The form is now:

Contour cmin cmax cstep [%] **[noline]**

The default contour plot will include black lines separating the contour colors. This can be turned off with the new "noline" keyword. The MCNP commands cmin, cmax, and cstep are the minimum, maximum, and step values for contours. The % will cause these to be interpreted as percentages. The default is 5 95 10 %.

6.4.3. Future Work

1. Extend 2D color tally contour plots to mesh tallies;

2. Sub-blocking (i.e., plotting sub-sections of the full contour plot) is performed with a standard contour plot; however this is currently disabled for specialized contour plots (i.e., free ij). The only drawback to this is that larger arrays are required to store the tally values (these can be quite large for a detailed contour plot, e.g. 1000x1000). To allow sub-blocking, additional logic is required in PLOTCN to sub-block on a full horizontal row at a time.
3. This contour upgrade allows for easy viewing of lattice tally data, but it is limited to look at 2-D slices in only one way for a full 3-D lattice. In this case, plots can only be in the "i" and "j" index plane, with "k" slices specified with the "fix" command. A user can not currently look at a "j" and "k" contour plot or a "i" and "k" contour plot. To allow this significant changes are required to subroutine EXTRCT which would enable the extraction of non-contiguous tally values.

The new plotting capabilities are accessible via either the interactive geometry plot capability or the command/prompt interface.

6.5. Proton and Photonuclear Cross-Section Plots

6.5.1. Photonuclear Cross-Section Plots

MCNPX can plot photonuclear data in addition to the photoatomic data of MCNP.

Photoatomic reaction numbers are all negative: -1 = incoherent, -2 = coherent, -3 = photoelectric, -4 = pair production, -5 = total, and -6 = heating. For the MCNPX photonuclear cross-section plotting, the reaction numbers are all positive. The principal photonuclear cross sections are as follows: 1 = total, 2 = nonelastic, 3 = elastic, 4 = heating, and >4 = various reactions such as 18 = (γ,f). The photonuclear yields (multiplicities) for various secondary particles are specified by adding 1000 times the secondary particle number to the reaction number. For example, 31001 is the total yield of deuterons (particle type d = 31); 34001 is the total yield of alphas (particle type α = 34); and 1018 is the total number of neutrons (particle type n = 1) from fission. To find out which reactions are available for a particular nuclide or material, enter an invalid reaction number, such as mt = 99, and MCNPX will list the available photonuclear reactions and the available yields such as 1018, 31018, 34018. Entering a bad nuclide, xs = 12345.67u, will cause MCNPX to list the available nuclides.

Figure 2 illustrates a photonuclear cross-section plot of the total photonuclear cross section, mt = 1, for material 11 and its constituents, carbon and lead.

6.5.2. Proton Cross-Section Plots

MCNPX NOW CAN PLOT PROTON CROSS SECTIONS. THE REACTION NUMBERS ARE SIMILAR TO THE NEUTRON REACTION NUMBERS: ALL POSITIVE. THE PRINCIPAL PROTON CROSS SECTIONS ARE THE FOLLOWING: ±1 = TOTAL, ±2 = NONELASTIC, ±3 = ELASTIC, ±4 = HEATING, AND >4 = VARIOUS REACTIONS. ON THE LA150H PROTON LIBRARY, THE ONLY AVAILABLE REACTION IS MT = 5 WITH ITS MULTIPLICITIES, 1005, 9005, 31005, ETC. THE MULTIPLICITY

REACTION NUMBERS FOR INTERACTION REACTION MT = 5 ARE 1005 FOR NEUTRONS, 9005 FOR PROTONS, 31005 FOR DEUTERONS, ETC. TO

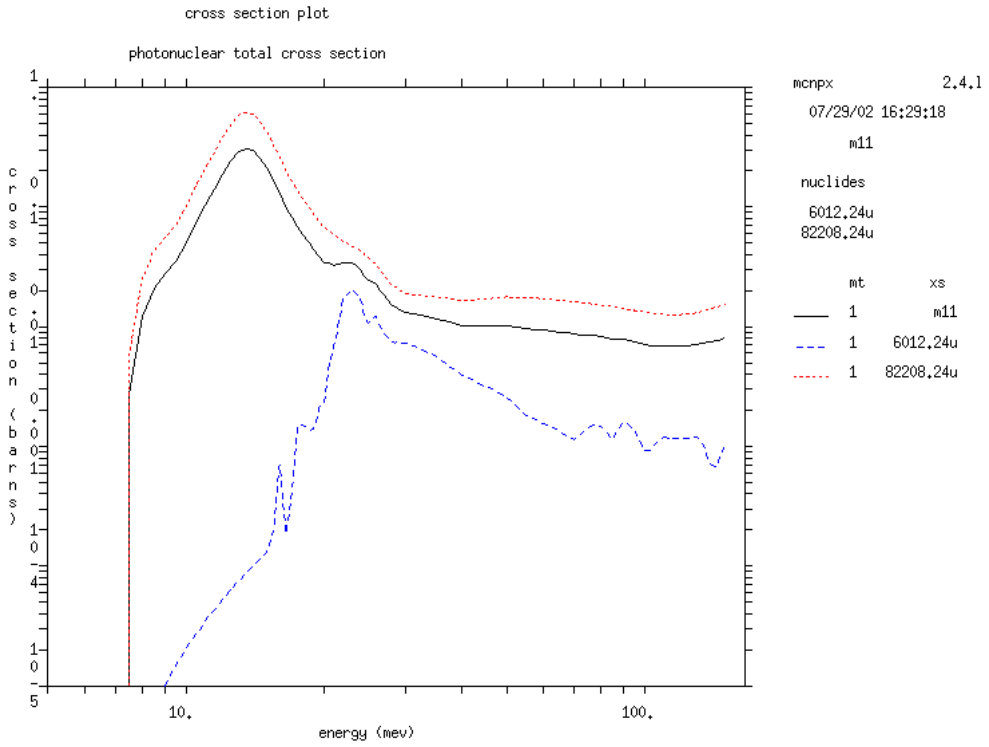


Fig. 2. Photonuclear cross-section plot.

find out which reactions are available for a particular nuclide or material, enter an invalid reaction number, such as mt = 99, and MCNPX will list the available proton reactions and the available yields such as 1005, 32001, and 34002. The proton multiplicity, mt = 9001, 9004, 9005, etc., is generally available, along with the total cross-section and heating number, mt = 1, mt = 4. Entering a bad nuclide, xs = 12345.67h, will cause MCNPX to list the available proton nuclides.

6.6. Pause Command

The MCNPX geometry plot *PAUSE* command now is extended to tally and cross-section plots. When the word *PAUSE N* is put in a tally plotting the COM input file, the picture will display for *N* seconds. If the command *PAUSE* (without the *N*) is in the COM file, the display will hold until a key is struck.

7.0. PARALLEL PROCESSING

- Distributed memory multiprocessing for all particles and energies;
- Message passing interface (MPI) multiprocessing;
- Significant speedup of criticality problems run with MPI.

7.1. Distributed Memory Multitasking for the Entire Energy Range of All Particles

The entire MCNPX code may be run in parallel using message passing. Table physics problems (i.e., standard MCNP4C3 problems) can be run with threading and/or message passing. Fault tolerance and load balancing are available, and multiprocessing can be done across a network of heterogeneous platforms. Parallel Virtual Machine (PVM) software or Message Passing Interface (MPI) software can be used.

The parallel message passing capability applies to all particles for their entire energy range and for all physics models.

7.2. MPI Multiprocessing

The Message Passing Interface (MPI) parallel communication software is now supported.

To compile MCNPX with MPI, it is necessary to use the new "MPILB" configuration option and provide a path to the MPI header file (this may not be necessary on some systems if these header files are already in the standard include path):

```
Configure –with-MPILIB[="/path/to/MPI/libraries  -lmpich"]
        --with –FFLAGS="-I/path/to/MPI/include/files"  .
```

To run an MCNPX problem with MPI, simply start the MPI daemon (which typically is running already on most systems) and then start MCNPX using "MPIRUN". An example is

```
mpirun -np 4 mcnpx inp=gwm na=gwm1. ...   .
```

This is quite different from the parallel virtual machine (PVM), which required knowledge about setting certain links, environment variables, and the PVM console commands. An example of the PVM execution command is

```
mcnpx inp=gwm n=gwm1. tasks=-12   .
```

See "installation notes for building MCNPX with MPI" on the MCNPX documents page, http://mcnpx.lanl.gov/documents.html .

7.3. MPI Speedup for Criticality Calculations

Note: This new capability speeds up MPI KCODE calculations but also has some collateral consequences for sequential KCODE calculations.

Criticality calculations (KCODE source) *will now run 10 – 1000 times faster* in parallel with MPI multiprocessing. The speedup depends upon the number of CPUs and the number of histories per cycle As the number of CPUs increases above ~8 and the histories per cycle approaches ~1M, the speedup quickly increases from a factor of ~10 to above 1000 with 64 CPUs.

The speedup has been achieved by having the next-generation fission source points on each processor stay on that processor No longer are the fission source points from all processors combined at the end of each cycle for rebroadcast the next cycle. The considerable expense of grouping the particles together at each processor rendezvous has been eliminated.

7.3.1. DXTRAN and Detector Tracking Differences

All calculations with DXTRAN and detectors --- not just KCODE or parallel calculations – generally no longer track Answers are still correct, but these next-event estimator problems do not track unless the 21st entry on the DBCN card is set nonzero or the default Russian roulette detector game (DD card) is not played The tracking difference is because the default Russian roulette game no longer adjusts the roulette criteria at the 200th history The Russian roulette criteria is still set at all tally fluctuation chart intervals, NPD, the 5th entry on the PRDMP card The default for NPD is still 1000 histories for fixed-source problems, but is now NPD = 1 (at the end of each cycle) for KCODE problems So a fixed-source problem that used to start playing Russian roulette on next-event estimates at history 200 now waits until history 1000.

7.3.2. User Interface Changes for both Sequential and Parallel KCODE Problems

The new method has consequences for both sequential and parallel KCODE calculations:

- Tally fluctuation charts are printed only at the ends of KCODE cycles rather than at specific particle intervals.
- The units for the fifth entry of the PRDMP card is changed for KCODE calculations The fifth entry is NPD, the tally fluctuation chart print interval For KCODE calculations, NPD is now the number of cycles (default = 1).
- KCODE problems with DXTRAN and point detectors are still correct, but may not track previous versions if the default Russian roulette game on small scores is played The tracking difference is because the roulette criteria is updated in different places DXTRAN and detectors utilizing negative DD card entries (to have a constant Russian roulette game criteria) still track.
- Setting the 21st entry on the DBCN card to 1 will cause MCNPX to track MCNPX 2.5.d without the new speedup capability:

```
DBCN  20J     1
```

7.3.3. User Interface Changes for Parallel KCODE Problems

- The KCODE speedup is only available for negative JTASKS: *tasks* = *-n x m* on the MCNPX execution line. Microtasking/load balancing (positive JTASKS) calculations use the slower former MCNP4C communication algorithm for KCODE source updating. A warning is issued if JTASKS > 0 in a KCODE calculation.
- In rare cases a subtask may deplete its source particles Only problem efficiency is affected and a warning is issued.

7.3.4. Compiler and Operating System Problems for Parallel KCODE Problems

- CTRL-C and quit on a multiple processor MPI run in Linux does not finish writing the OUTP file before MCNPX exits. This failure appears to be an MPI error (possibly feature) in the MPI_FINALIZE call where the last processor kills all subtasks and the master.
- CTRL-C interrupt does not function properly in Windows 2000 (probably general to all Windows). The user can attempt to quit but MCNPX will hang and the user will be forced to kill the process through multiple CTRL-C commands.
- The Portland Group pgcc compiler (version 4.02) will not properly compile the ANL mpich-1.2.5 on a Linux system. However GCC 3.2.3 will work to build the MPICH libraries.

8.0. COMPILING, CONFIGURATION, AND INSTALLATION

- FORTRAN90 modularity and dynamic memory allocation;
- F90 autoconfiguration;
- 64-bit integer support;
- NAG/IBM/INTEL compiler extensions.

8.1. FORTRAN 90 Modularity and Dynamic Memory Allocation

The F90 conversion provides improvements in code modularity, standardization of functions such as timing across platforms, and compiler reliability. F90 will run more slowly on some systems. Specifically, we have eliminated equivalences as a means of dynamic storage allocation by using F90 pointers and allocable arrays. We have replaced most common calls with F90 modules. The code will compile in both free and fixed F90 formats.

MCNPX can be modified by patches, and as much of the MCNP4C coding as possible has been preserved so that MCNP4C patches can be applied directly to MCNPX.

Continuing improvements in the F90 structure are ongoing, especially where they concern physics modules that have been brought into the code.

8.2. F90 Autoconfiguration

MCNPX has a unique autoconfiguration build system which allows a variety of compilation options to be easily executed on a large number of platforms. MCNPX supports Linux, Windows PC, Sun Solaris unix, HPUX unix, IBM AIX unix, and SGI unix.

Test problems and their solution templates are available for all supported systems. The 65 test problems consist of the 42-problem MCNP5 test set supplemented by 23 problems testing MCNPX exclusive features. The test problems on all systems can be run and compared against the solution templates with a single simple in autoconfigureation comand.

8.3. 64-bit Integer Support

MCNPX has been restructured to enable 64-bit integers MCNP and MCNPX have always had 64-bit floating point reals either by use of compiler directives on supercomputers or by double precision on “cheap” computers (most systems.) But the integers have been 4-byte (32-bit)on all

but a few supercomputers; this limits the number of histories that can be run to about 2 billion. It also limits the amount of cross sections and tallies in a problem because these use integer pointers.

With the 64-bit integer capability you can run up to 1e18 histories. You can avoid memory access problems and have nearly all the cross sections and tallies you want.

The print field for the number of histories run in a problem has been increased to 12 digits to accommodate the long runs now possible with parallel processing.

8.3.1. Recompilation Requirements for 64-bit Integers

The default for MCNPX is still 4-byte integers. The executable versions provided on the MCNPX Beta Test page are all 4-byte integer versions To use the 64-bit version it is necessary to

1. recompile with special options; and
2. either use type-1 ascii cross section tables or rebuild your type-2 binary cross section tables using 64-bit integer pointers using MAKXS.

If you generally recompile your own MCNPX versions and use type-1 ascii cross sections you can go to the 64-bit integers rather easily. When you configure, simply use the options:

--with-FFLAGS=-i8 –with-NOCHEAP

The –with-NOCHEAP directive is not available on all systems If it is not recognized on your system then add the compile directive

--with-FFLAGS=-i8

and remove –DCHEAP=1 from src/mcnpx/mcnpf/Makefile.h.

The 64-bit integer capability is unavailable on PCs. The –i8 compile option is not available on the CVF Fortran 90 compiler and possibly other compilers. The 64-bit integers will increase the size of the code.

8.3.2. Additional Notes

The 64-bit integer capability was an extensive change to MCNPX because it affected most Fortran 90 “kind” specifications. We also eliminated all “REAL” declarations where floating point variables went to different default (usually 32-bit) lengths on various systems. A consequence is that real variables are all 64-bit unless some other length is required for interfaces to plotting or interrupts or other special purposes. The tracking between different compilers and platforms is now more consistent. Finally, this capability made extension to new compilers and platforms (see next Section) easier.

8.4. NAG/IBM/INTEL F90 and Compiler Extensions

MCNPX now runs on a wider variety of platforms and operating systems by utilizing more standard Fortran 90 constructs and some fairly extensive code and autoconfiguration changes In particular, it runs on the G5 OS X system using the NAG 4.2 compiler for the Apple Power Mac G5. MCNPX also runs on this platform with the IBM compiler.

The NAG compiler passes the SGI test suite on the Mac with "-O1" optimization The IBM compiler passes with "-O2" optimization and is 17% faster. A trial version of the IBM compiler is available from http://www.ibm.com/ ; see support & downloads --- trials & betas A-Z --- XL Fortran.

There is no MCNPX parallel capability yet for the NAG compiler.

9.0. SUMMARY OF MCNPX CAPABILITIES SINCE MCNP4B BY VERSION

The extensions of MCNPX beyond MCNP4B are now listed according to version release with the initials of the principal developers shown in parentheses.[6]

MCNPX 2.5.e (February 2004)

-
- 2D color tally contour plots, including lattices and radiography (GWM)
- Significant speedup of criticality problems run with MPI (GWM/NAC)
- 64-bit integer support (GWM)
- NAG/IBM/INTEL compiler extensions
- Photon Doppler broadening (from MCNP5) (AS)

MCNPX 2.5.d (August 2003)

- INCL4/ABLA physics models (JCD/JSH);
- Lattice tally speedup (GWM);
- Auxiliary input files: READ (JSH);
- Geometry plot of weight window generator superimposed mesh (JSH);
- Pulse height light tally with anticoincidence: FT8 PHL (GWM);
- Coincidence capture tally & PTRAC file: FT8 CAP (MTS/SJT/DRM/JSH);
- Residual nuclei tally: FT8 RES (JSH);
- Inline generation of double differential cross sections and residuals (JSH);
-

MCNPX 2.5.c (April 2003)

- message passing interface (MPI) multiprocessing (JL/GWM);

[6] Kenneth J. Adams (KJA), Nate A. Carstens (NAC), Leland L. Carter (LLC), Skip Egdorf (HWE), Thomas M. Evans (TME), Jeffrey A. Favorite (JAF), Franz X. Gallmeier (FXG), John S. Hendricks (JSH), H. Grady Hughes (HGH), Julian Lebenhaft (JL), Robert C. Little (RCL), Stepan G. Mashnik (SGM), Gregg W. McKinney (GWM), Eric J. Pitcher (EJP), Richard E. Prael (REP), Teresa L. Roberts (TLR), Arnold J. Sierk (AJS), Edward C. Snow (ECS), Avneet Sood (AS), Laurie S. Waters (LSW), Christopher J. Werner (CJW), and Morgan C. White (MCW).

- i,j,k lattice indexing in geometry plots (JSH),
- enable of weight-window generator in physics model region (FXG/ JSH);
- enablement of exponential transform in physics model region (FXG/JSH);
- extension of neutron model physics below 20 MeV (JSH);
- ^{3}He coincidence detector modeling (HGH/JSH);
- F90 autoconfiguration (TLR)

MCNPX 2.5.b (November 2002)

- CEM2k physics (SGM/AJS/FXG);
- mix and match (JSH);
- positron sources (HGH);
- spontaneous fission (JSH)

MCNPX 2.4.0 (August 2002)

- FORTRAN90 modularity and dynamic memory allocation (GWM);
- distributed memory multiprocessing for the entire energy range of all particles (GWM);
- repeated structures source-path improvement (LLC/JSH);
- default dose functions (LSW/JSH);
- light-ion recoil (JSH);
- enhanced color geometry plots (GWM/JSH);
- photonuclear cross-section plots (JSH);
- proton cross-section plots (JSH);
- proton reaction multipliers with FM cards (JSH);
- photonuclear reaction multipliers with FM cards (JSH/GWM);
- some speedups (GWM/JSH);
- logarithmic interpolation on input cards (JSH);
- cosine bins that may be specified in degrees (JSH);
- cosine bins that may be specified for F2 flux tallies (JSH);
- source particles that may be specified by descriptors (JSH);
- pause command for tally and cross-section plots (JSH).

MCNPX 2.3.0 and previous MCNPX versions (1995–2001)

- physics for 34 particle types (HGH);
- high-energy physics above the tabular data range (REP);
- photonuclear physics (MCW);
- neutron, proton, and photonuclear 150-MeV libraries and utilization (RCL);
- mesh tallies (tallies in a superimposed mesh) (LSW/ECS);
- radiography tallies (JSH/ECS);
- secondary-particle production biasing (ECS); and
- autoconfiguration build system for compilation (TLR/HWE).
-

MCNP4C3, MCNP4C2, and MCNP4C features added after MCNP4B (1997–2001)

- PC enhancements: Linux and Windows capable (LLC/GWM);
- easier geometry specification with macrobodies (LLC);
- interactive geometry plotting (JSH);
- improved variance reduction with the superimposed mesh weight-window generator (TME/JAF/JSH);
- superimposed mesh plotting (JSH);
- delayed neutrons (CJW);
- unresolved resonance range probability tables (LLC/RCL);
- perturbations for material-dependent tallies (GWM/LLC/JSH);
- ENDF/B-VI extensions (MCW);
- electron physics enhancements (upgrade to ITS3.0)[7] (KJA/HGH);
- weight-window enhancements (JSH/JAF); and
- distributed memory multiprocessing (GWM).

10.0. FUTURE WORK

- Pulse-height tallies with variance reduction
- Mesh tally contour plotting
- Cinder90 capabilities
  - Delayed neutrons physics models
  - Delayed gamma physics models
  - Transmutation
- Criticality
  - Externally driven sources
  - Improved stability of eigenfunctions
- Plotting of physics model total and absorption cross sections
- Forced collisions for neutral particles extended to physics models
- Improved high-energy physics with the LAQGSM model
- Secondary particle angle biasing for isotropic distributions
- Neutral particle perturbation techniques extended to physics model region
- Heavy-ion tracking and interactions
- Detectors and DXTRAN for all neutral particles at all energy ranges
- A capability to continue runs that write HTAPE files
- Interactive tally and cross-section plotting
- Integration of HTAPE tallies directly into MCNPX
- CAD link
- Magnetic field tracking.

[7] J. A. Halbleib, R. P. Kensek, T. A. Mehlhorn, G. D. Valdez, S. M. Seltzer, M. J. Berger, "ITS Version 3.0: The Integrated TIGER Series of Coupled Electron/Photon Monte Carlo Transport Codes," Sandia National Laboratories report SAND91-1634 (March 1992).

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